



Full wwPDB EM Validation Report ⓘ

Mar 27, 2026 – 12:22 PM UTC

PDB ID : 6R7Q / pdb_00006r7q
EMDB ID : EMD-4745
Title : Structure of XBP1u-paused ribosome nascent chain complex with Sec61.
Authors : Shanmuganathan, V.; Cheng, J.; Braunger, K.; Berninghausen, O.; Beatrix, B.; Beckmann, R.
Deposited on : 2019-03-29
Resolution : 3.90 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

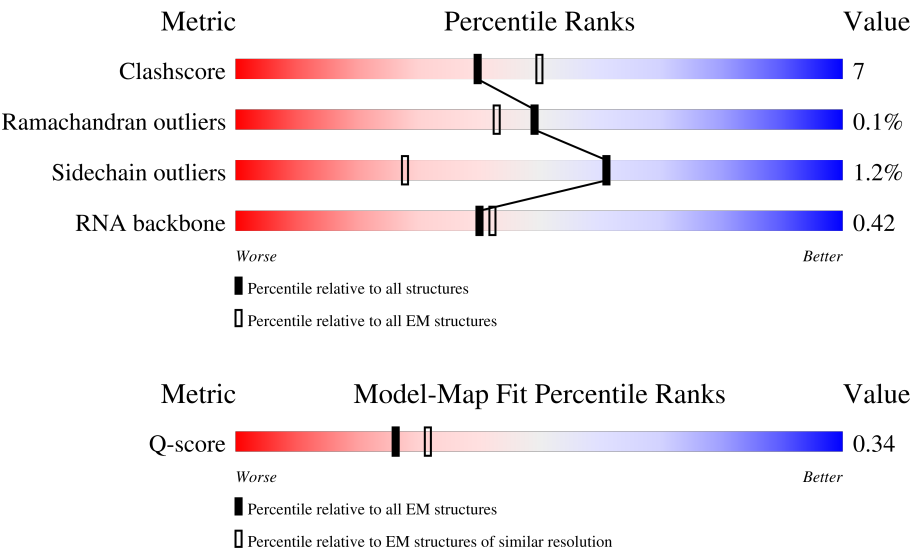
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	8855 (3.40 - 4.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AA	55	
2	BB	189	
3	CC	206	

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Mol	Chain	Length	Quality of chain
4	DD	185	
5	EE	151	
6	FF	62	
7	GG	100	
8	HH	83	
9	II	144	
10	JJ	83	
11	KK	132	
12	LL	101	
13	MM	136	
14	0	68	
15	1	24	
16	2	75	
17	3	75	
18	4	6	
19	5	3544	
20	6	313	
21	7	120	
22	8	151	
23	9	55	
24	NN	124	
25	OO	75	
26	PP	141	
27	QQ	149	
28	RR	117	

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Mol	Chain	Length	Quality of chain
29	A	248	
30	B	394	
31	C	362	
32	D	293	
33	E	251	
34	F	225	
35	G	240	
36	H	190	
37	I	213	
38	J	170	
39	K	1698	
40	L	210	
41	M	138	
42	N	203	
43	O	199	
44	P	153	
45	Q	187	
46	R	180	
47	S	176	
48	T	159	
49	U	99	
50	V	131	
51	W	121	
52	X	118	
53	Y	134	

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Mol	Chain	Length	Quality of chain
54	Z	135	
55	SS	96	
56	a	147	
57	b	116	
58	c	98	
59	d	107	
60	e	128	
61	f	109	
62	g	114	
63	h	122	
64	i	102	
65	j	86	
66	k	69	
67	l	50	
68	m	52	
69	n	25	
70	o	104	
71	p	91	
72	q	217	
73	r	124	
74	s	196	
75	t	153	
76	u	213	
77	v	221	
78	w	228	

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Mol	Chain	Length	Quality of chain
79	x	262	
80	y	191	
81	z	237	
82	TT	129	
83	UU	142	
84	VV	141	
85	WW	120	
86	XX	461	
87	YY	62	
88	ZZ	29	

2 Entry composition

There are 90 unique types of molecules in this entry. The entry contains 219898 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AA	55	Total	C	N	O	S	0	0
			443	274	97	71	1		

- Molecule 2 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	BB	185	Total	C	N	O	S	0	0
			1488	952	271	264	1		

- Molecule 3 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	CC	206	Total	C	N	O	S	0	0
			1686	1058	332	291	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CC	47	ARG	GLY	conflict	UNP G1TJW1

- Molecule 4 is a protein called Ribosomal protein S9 (Predicted).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	DD	185	Total	C	N	O	S	0	0
			1525	969	306	248	2		

- Molecule 5 is a protein called Ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	EE	143	Total	C	N	O	S	0	0
			1175	749	222	198	6		

- Molecule 6 is a protein called Ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	FF	62	Total	C	N	O	S	0	0
			488	297	97	92	2		

- Molecule 7 is a protein called uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	GG	100	Total	C	N	O	S	0	0
			795	498	152	141	4		

- Molecule 8 is a protein called eS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	HH	83	Total	C	N	O	S	0	0
			636	393	117	121	5		

- Molecule 9 is a protein called uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	II	144	Total	C	N	O	S	0	0
			1190	746	241	202	1		

- Molecule 10 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	JJ	83	Total	C	N	O	S	0	0
			651	408	121	115	7		

- Molecule 11 is a protein called eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	KK	132	Total	C	N	O	S	0	0
			1068	670	199	195	4		

- Molecule 12 is a protein called eS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	LL	101	Total	C	N	O	S	0	0
			814	507	170	132	5		

- Molecule 13 is a protein called uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	MM	136	Total	C	N	O	S	0	0
			1016	621	199	190	6		

- Molecule 14 is a protein called eS31.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	0	68	Total	C	N	O	S	0	0
			555	351	103	94	7		

- Molecule 15 is a protein called X-box-binding protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	1	24	Total	C	N	O	S	0	0
			204	137	35	30	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	255	ALA	SER	conflict	UNP P17861

- Molecule 16 is a RNA chain called P-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	2	75	Total	C	N	O	P	0	0
			1594	713	285	522	74		

- Molecule 17 is a RNA chain called E-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	3	75	Total	C	N	O	P	0	0
			1597	714	287	522	74		

- Molecule 18 is a RNA chain called messenger RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	4	6	Total	C	N	O	P	0	0
			127	57	21	43	6		

- Molecule 19 is a RNA chain called 28S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	5	3543	Total	C	N	O	P	0	0
			75972	33833	13910	24686	3543		

- Molecule 20 is a protein called ribosomal protein RACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	6	313	Total	C	N	O	S	0	0
			2436	1535	424	465	12		

- Molecule 21 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	7	120	Total	C	N	O	P	0	0
			2558	1141	456	842	119		

- Molecule 22 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	8	151	Total	C	N	O	P	0	0
			3208	1432	564	1062	150		

- Molecule 23 is a protein called uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	9	55	Total	C	N	O	S	0	0
			459	286	94	74	5		

- Molecule 24 is a protein called eS24.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	NN	124	Total	C	N	O	S	0	0
			1011	640	198	168	5		

- Molecule 25 is a protein called ribosomal protein eS25.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	OO	75	Total	C	N	O	S	0	0
			598	382	111	104	1		

- Molecule 26 is a protein called eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	PP	141	Total	C	N	O	S	0	0
			1097	688	211	195	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
PP	119	GLY	TRP	conflict	UNP G1TN62

- Molecule 27 is a protein called ribosomal protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	QQ	149	Total	C	N	O	S	0	0
			1202	770	228	203	1		

- Molecule 28 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	RR	117	Total	C	N	O	S	0	0
			908	570	161	169	8		

- Molecule 29 is a protein called uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	A	248	Total	C	N	O	S	0	0
			1898	1189	389	314	6		

- Molecule 30 is a protein called uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	B	394	Total	C	N	O	S	0	0
			3172	2020	597	542	13		

- Molecule 31 is a protein called uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	C	362	Total	C	N	O	S	0	0
			2883	1812	577	480	14		

- Molecule 32 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	D	293	Total	C	N	O	S	0	0
			2391	1512	438	427	14		

- Molecule 33 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	E	216	Total	C	N	O	S	0	0
			1729	1115	329	282	3		

- Molecule 34 is a protein called uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	F	225	Total	C	N	O	S	0	0
			1875	1205	358	303	9		

- Molecule 35 is a protein called eL8.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	G	233	Total	C	N	O	S	0	0
			1879	1199	361	315	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	244	GLY	CYS	conflict	UNP G1STW0

- Molecule 36 is a protein called uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	H	190	Total	C	N	O	S	0	0
			1516	954	284	272	6		

- Molecule 37 is a protein called Ribosomal protein L10 (Predicted).

Mol	Chain	Residues	Atoms					AltConf	Trace
37	I	205	Total	C	N	O	S	0	0
			1664	1056	321	274	13		

- Molecule 38 is a protein called Ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	J	170	Total	C	N	O	S	0	0
			1362	861	254	241	6		

- Molecule 39 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	K	1698	Total	C	N	O	P	0	0
			36249	16180	6508	11864	1697		

- Molecule 40 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	L	210	Total	C	N	O	S	0	0
			1702	1065	354	279	4		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	47	ALA	-	insertion	UNP G1TPV0
L	48	PRO	-	insertion	UNP G1TPV0
L	49	ARG	-	insertion	UNP G1TPV0
L	50	PRO	-	insertion	UNP G1TPV0
L	51	ALA	-	insertion	UNP G1TPV0
L	52	ALA	-	insertion	UNP G1TPV0
L	53	GLY	-	insertion	UNP G1TPV0
L	54	PRO	-	insertion	UNP G1TPV0
L	55	ILE	-	insertion	UNP G1TPV0

- Molecule 41 is a protein called Ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	M	138	Total	C	N	O	S	0	0
			1137	727	221	182	7		

- Molecule 42 is a protein called Ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	N	203	Total	C	N	O	S	0	0
			1701	1072	359	266	4		

- Molecule 43 is a protein called uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	O	199	Total	C	N	O	S	0	0
			1630	1051	319	255	5		

- Molecule 44 is a protein called uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	P	153	Total	C	N	O	S	0	0
			1242	777	241	215	9		

- Molecule 45 is a protein called eL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	Q	187	Total	C	N	O	S	0	0
			1515	946	315	250	4		

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	6	ARG	LEU	conflict	UNP G1TX70
Q	14	ARG	TRP	conflict	UNP G1TX70
Q	23	ILE	MET	conflict	UNP G1TX70
Q	24	TYR	CYS	conflict	UNP G1TX70
Q	38	ARG	HIS	conflict	UNP G1TX70
Q	57	ASN	LYS	conflict	UNP G1TX70
Q	66	MET	VAL	conflict	UNP G1TX70
Q	74	GLY	ASP	conflict	UNP G1TX70
Q	75	ARG	PRO	conflict	UNP G1TX70
Q	86	VAL	ILE	conflict	UNP G1TX70
Q	110	ARG	HIS	conflict	UNP G1TX70
Q	117	GLY	GLU	conflict	UNP G1TX70
Q	124	ASP	HIS	conflict	UNP G1TX70
Q	150	ARG	GLN	conflict	UNP G1TX70
Q	172	ARG	GLY	conflict	UNP G1TX70
Q	184	ARG	TRP	conflict	UNP G1TX70

- Molecule 46 is a protein called eL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	R	180	Total	C	N	O	S	0	0
			1508	933	328	238	9		

- Molecule 47 is a protein called eL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	S	176	Total	C	N	O	S	0	0
			1462	930	285	236	11		

- Molecule 48 is a protein called eL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	T	159	Total	C	N	O	S	0	0
			1298	823	252	217	6		

- Molecule 49 is a protein called eL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	U	99	Total	C	N	O	S	0	0
			809	519	141	147	2		

- Molecule 50 is a protein called eL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	V	131	Total	C	N	O	S	0	0
			979	618	184	172	5		

- Molecule 51 is a protein called Ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	W	106	Total	C	N	O	S	0	0
			860	538	174	144	4		

- Molecule 52 is a protein called uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	X	118	Total	C	N	O	S	0	0
			967	618	181	167	1		

- Molecule 53 is a protein called Ribosomal protein L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	Y	134	Total	C	N	O	S	0	0
			1115	700	226	186	3		

- Molecule 54 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	Z	135	Total	C	N	O	S	0	0
			1107	714	208	182	3		

- Molecule 55 is a protein called eS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	SS	96	Total	C	N	O	S	0	0
			810	530	143	131	6		

- Molecule 56 is a protein called uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	a	147	Total	C	N	O	S	0	0
			1162	734	239	185	4		

- Molecule 57 is a protein called eL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	b	104	Total	C	N	O	S	0	0
			848	527	189	129	3		

- Molecule 58 is a protein called eL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	c	98	Total	C	N	O	S	0	0
			761	481	134	140	6		

- Molecule 59 is a protein called eL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	d	107	Total	C	N	O	S	0	0
			888	560	171	155	2		

- Molecule 60 is a protein called eL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	e	128	Total	C	N	O	S	0	0
			1053	667	216	165	5		

- Molecule 61 is a protein called eL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	f	109	Total	C	N	O	S	0	0
			876	555	174	143	4		

- Molecule 62 is a protein called eL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	g	114	Total	C	N	O	S	0	0
			906	566	187	147	6		

- Molecule 63 is a protein called uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	h	122	Total	C	N	O	S	0	0
			1013	640	204	168	1		

- Molecule 64 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	i	102	Total	C	N	O	S	0	0
			830	520	176	129	5		

- Molecule 65 is a protein called Ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	j	86	Total	C	N	O	S	0	0
			705	434	155	111	5		

- Molecule 66 is a protein called eL38.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	k	69	Total	C	N	O	S	0	0
			569	366	103	99	1		

- Molecule 67 is a protein called eL39.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	l	50	Total	C	N	O	S	0	0
			447	286	96	64	1		

- Molecule 68 is a protein called eL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	m	52	Total	C	N	O	S	0	0
			429	266	90	67	6		

- Molecule 69 is a protein called 60s ribosomal protein l41.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	n	25	Total	C	N	O	S	0	0
			239	145	64	27	3		

- Molecule 70 is a protein called eL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	o	104	Total	C	N	O	S	0	0
			851	533	174	138	6		

- Molecule 71 is a protein called ribosomal protein eL43.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	p	91	Total	C	N	O	S	0	0
			708	445	136	120	7		

- Molecule 72 is a protein called uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	q	217	Total	C	N	O	S	0	0
			1710	1086	300	316	8		

- Molecule 73 is a protein called eL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	r	124	Total	C	N	O	S	0	0
			994	616	205	167	6		

- Molecule 74 is a protein called 60S acidic ribosomal protein P0.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	s	196	Total	C	N	O	S	0	0
			1507	959	263	276	9		

- Molecule 75 is a protein called uL11.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	t	153	Total	C	N	O	S	0	0
			1160	722	218	217	3		

- Molecule 76 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	u	213	Total	C	N	O	S	0	0
			1729	1098	309	308	14		

- Molecule 77 is a protein called uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	v	221	Total	C	N	O	S	0	0
			1716	1111	295	301	9		

- Molecule 78 is a protein called Ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	w	228	Total	C	N	O	S	0	0
			1768	1126	318	316	8		

- Molecule 79 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	x	262	Total	C	N	O	S	0	0
			2076	1324	386	358	8		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
x	25	GLY	SER	conflict	UNP G1TK17
x	51	ARG	LYS	conflict	UNP G1TK17
x	78	THR	ALA	conflict	UNP G1TK17
x	156	VAL	MET	conflict	UNP G1TK17

- Molecule 80 is a protein called Ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	y	185	Total	C	N	O	S	0	0
			1471	921	277	266	7		

- Molecule 81 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	z	237	Total	C	N	O	S	0	0
			1923	1200	387	329	7		

- Molecule 82 is a protein called Ribosomal protein S15a.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	TT	129	Total	C	N	O	S	0	0
			1034	659	193	176	6		

- Molecule 83 is a protein called Ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	UU	142	Total	C	N	O	S	0	0
			1128	717	213	195	3		

- Molecule 84 is a protein called Ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	VV	141	Total	C	N	O	S	0	0
			1098	693	219	183	3		

- Molecule 85 is a protein called uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
85	WW	120	Total	C	N	O	S	0	0
			997	635	187	168	7		

- Molecule 86 is a protein called Protein transport protein Sec61 subunit alpha isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
86	XX	426	Total	C	N	O	S	0	0
			3313	2181	535	576	21		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
XX	145	SER	THR	conflict	UNP P38377

- Molecule 87 is a protein called Protein transport protein Sec61 subunit gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
87	YY	62	Total	C	N	O	S	0	0
			494	326	86	79	3		

- Molecule 88 is a protein called Protein transport protein Sec61 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
88	ZZ	29	Total	C	N	O	S	0	0
			229	157	36	34	2		

- Molecule 89 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
89	LL	1	Total	Zn	0
			1	1	
89	g	1	Total	Zn	0
			1	1	
89	j	1	Total	Zn	0
			1	1	
89	m	1	Total	Zn	0
			1	1	
89	o	1	Total	Zn	0
			1	1	
89	p	1	Total	Zn	0
			1	1	

- Molecule 90 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
90	5	201	Total	Mg	0
			201	201	
90	7	7	Total	Mg	0
			7	7	
90	8	4	Total	Mg	0
			4	4	
90	B	1	Total	Mg	0
			1	1	
90	K	78	Total	Mg	0
			78	78	
90	P	2	Total	Mg	0
			2	2	
90	V	1	Total	Mg	0
			1	1	

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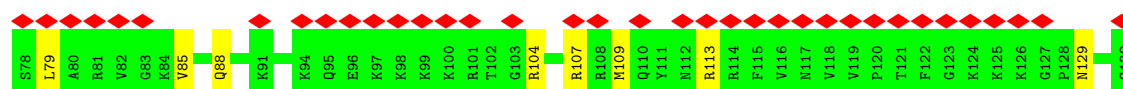
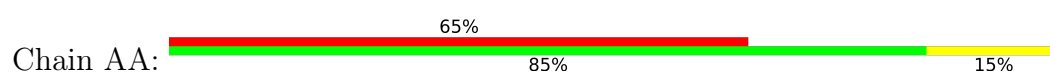
Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
90	a	1	Total 1	Mg 1	0
90	e	1	Total 1	Mg 1	0
90	g	1	Total 1	Mg 1	0
90	j	1	Total 1	Mg 1	0
90	y	1	Total 1	Mg 1	0

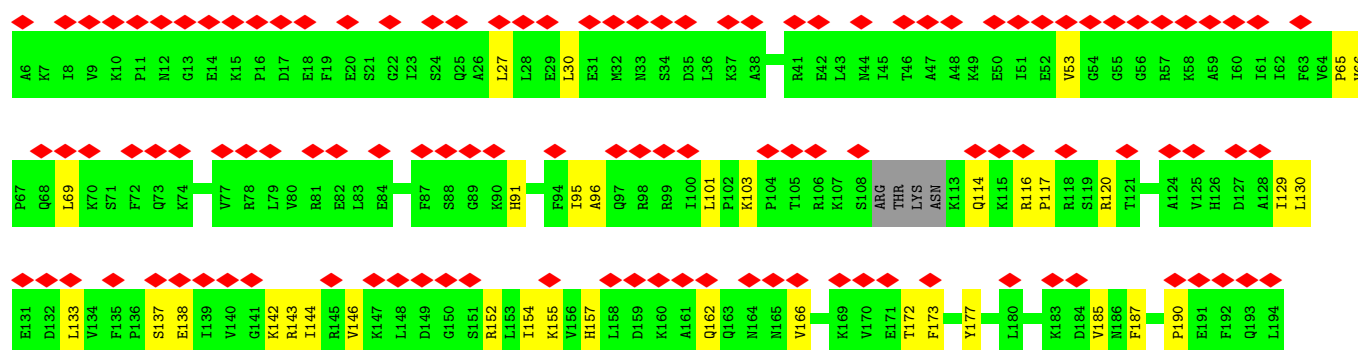
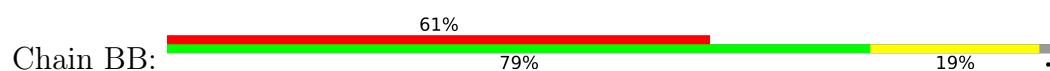
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

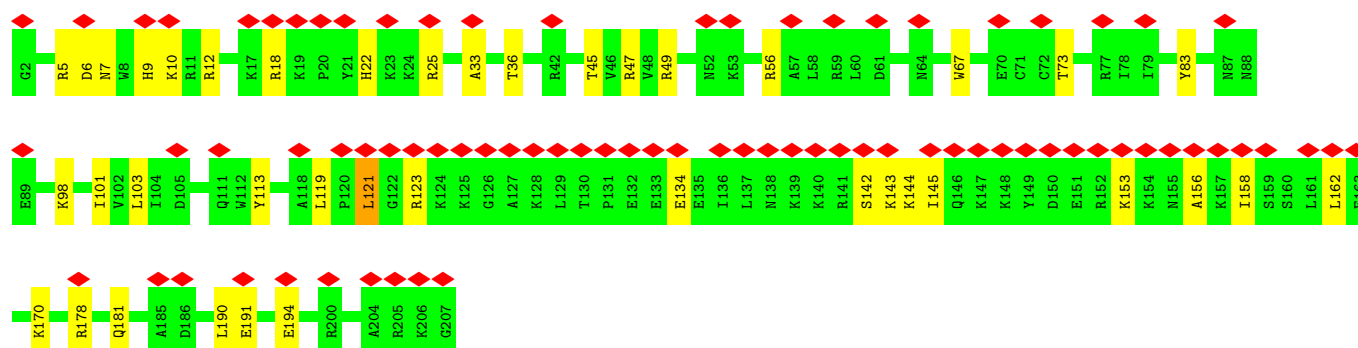
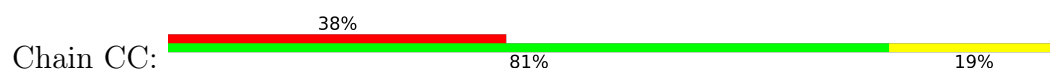
• Molecule 1: 40S ribosomal protein S30



• Molecule 2: 40S ribosomal protein S7

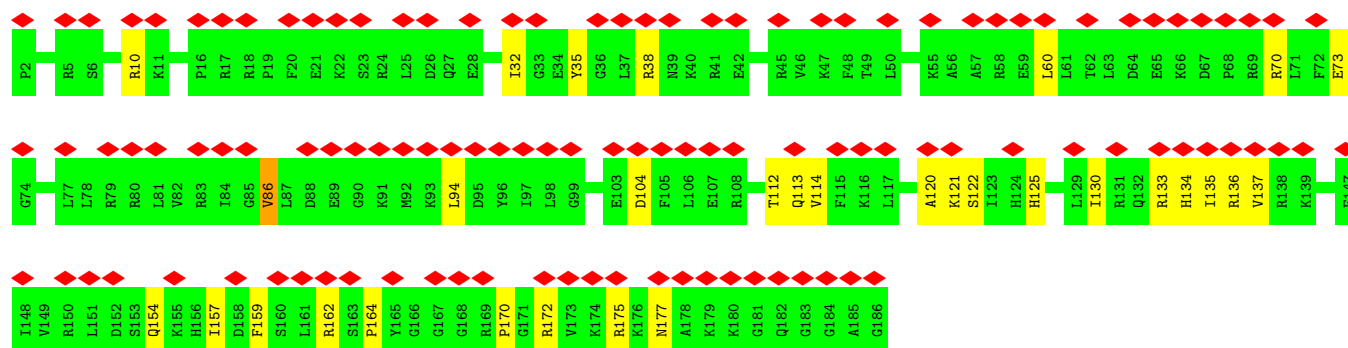


• Molecule 3: 40S ribosomal protein S8



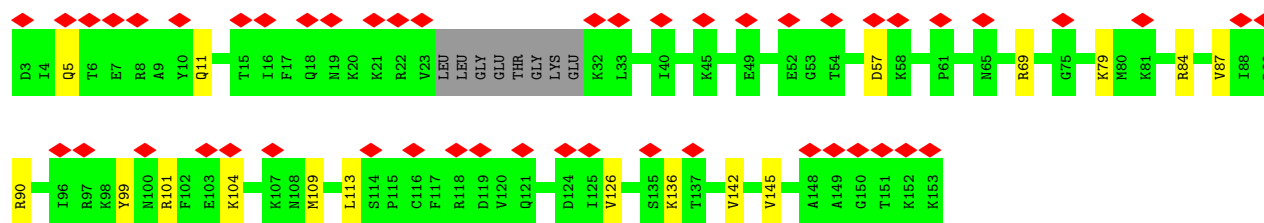
- Molecule 4: Ribosomal protein S9 (Predicted)

Chain DD: 

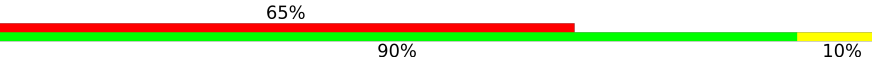


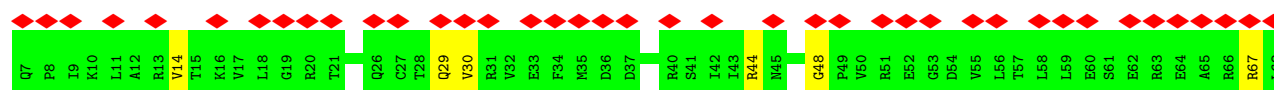
- Molecule 5: Ribosomal protein S11

Chain EE: 



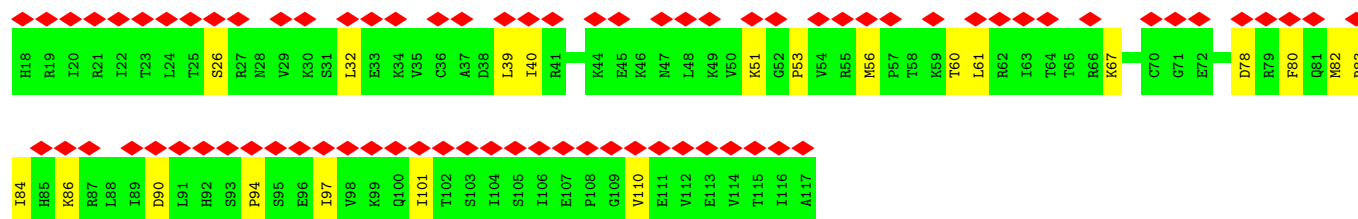
- Molecule 6: Ribosomal protein S28

Chain FF: 



- Molecule 7: uS10

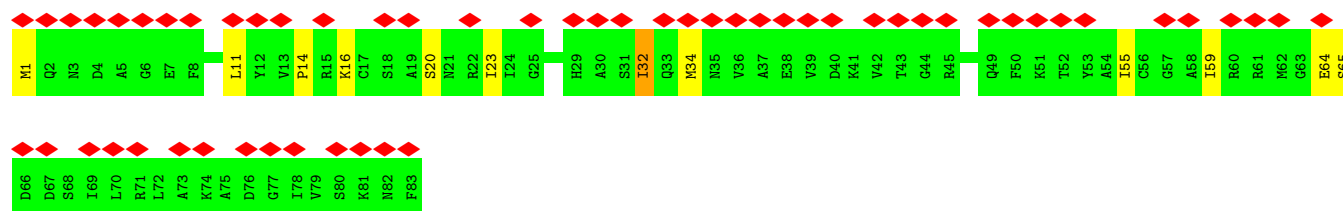
Chain GG: 



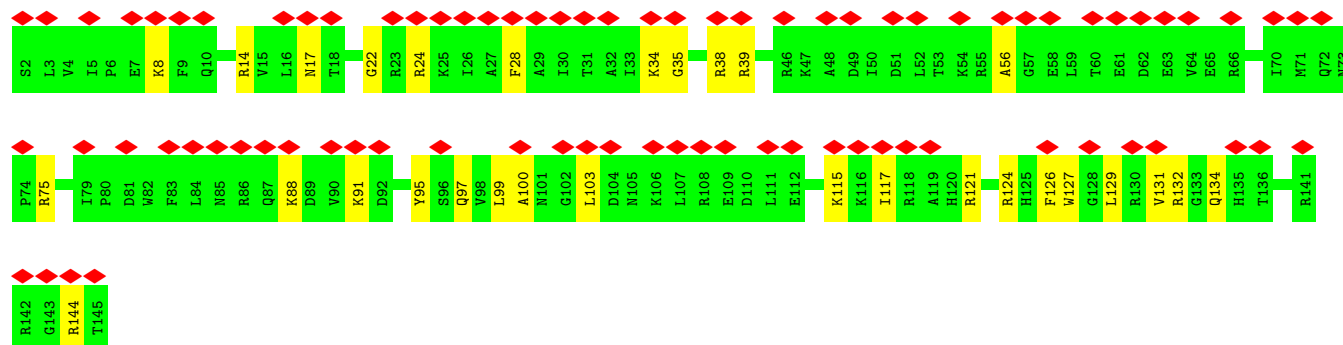
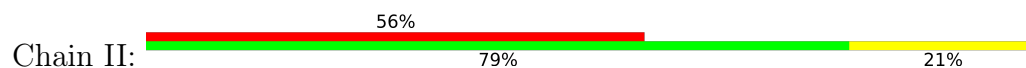
- Molecule 8: eS21

Chain HH: 

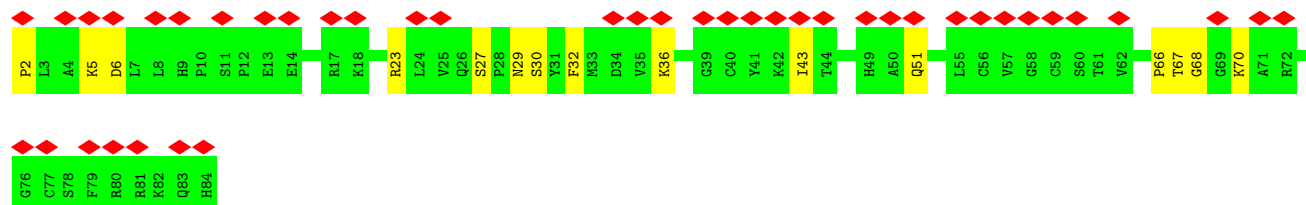
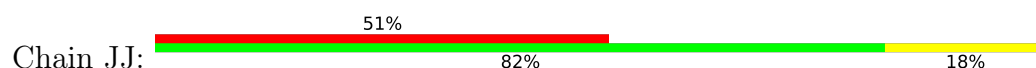




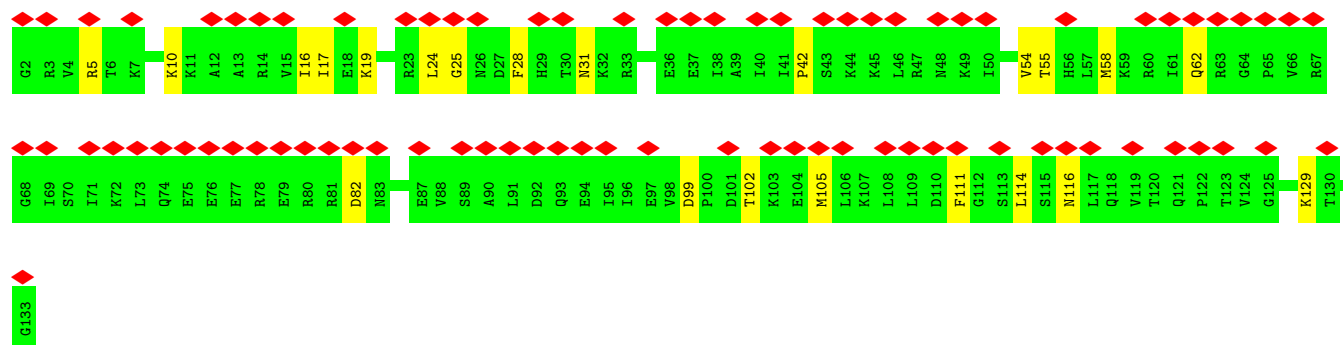
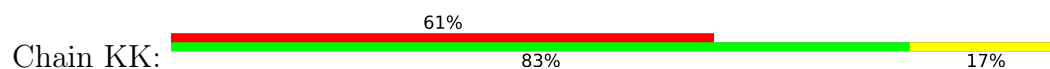
• Molecule 9: uS13



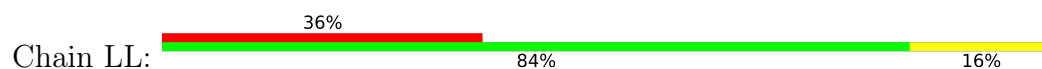
• Molecule 10: 40S ribosomal protein S27

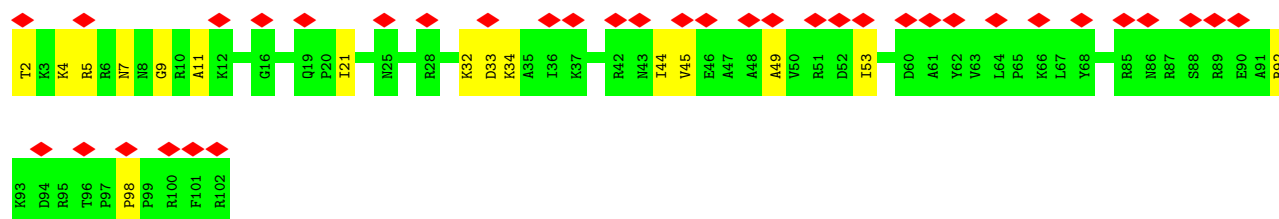


• Molecule 11: eS17

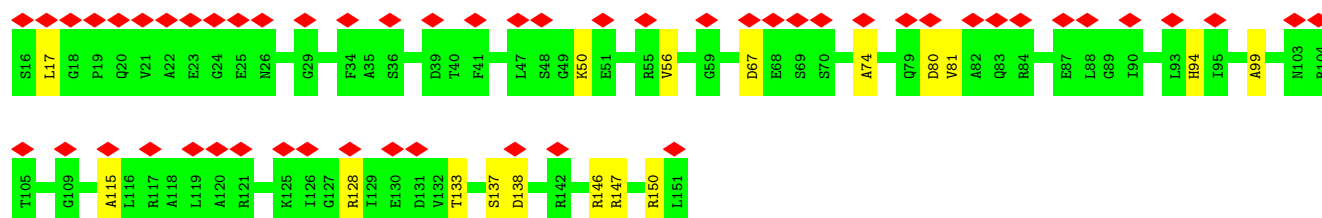
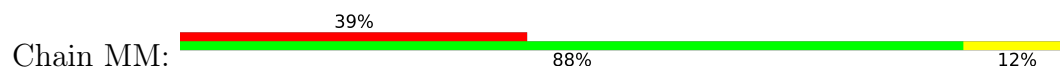


• Molecule 12: eS26

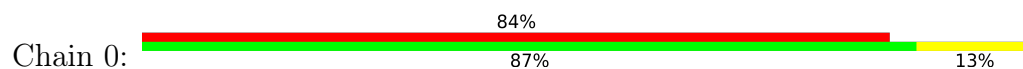




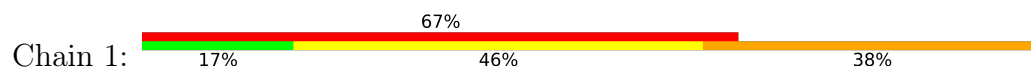
- Molecule 13: uS11



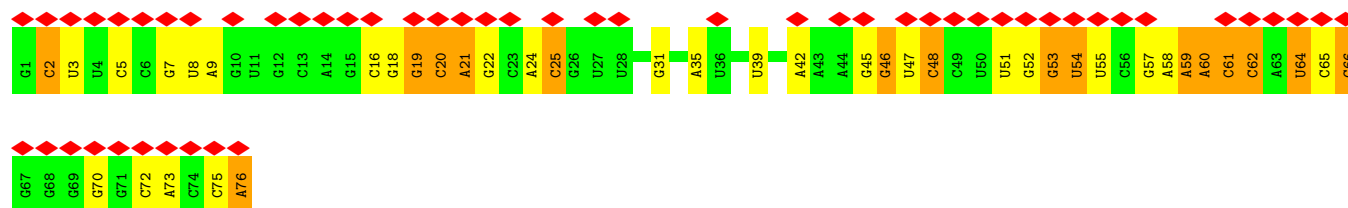
- Molecule 14: eS31



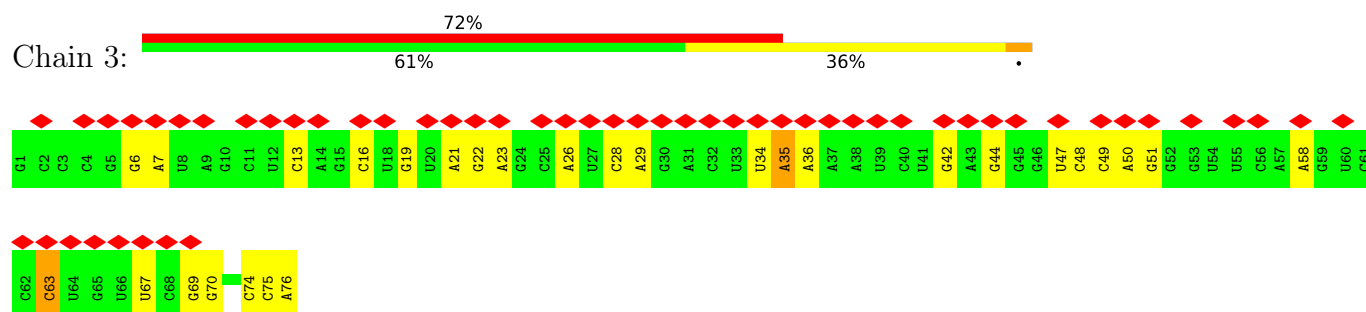
- Molecule 15: X-box-binding protein 1



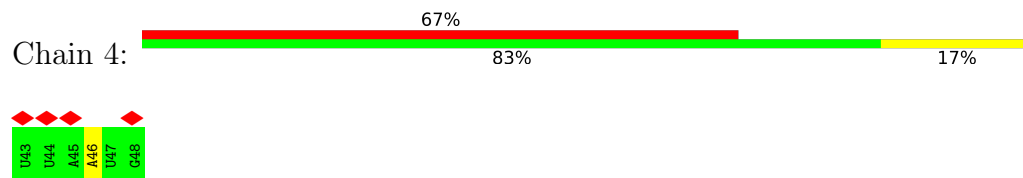
- Molecule 16: P-tRNA



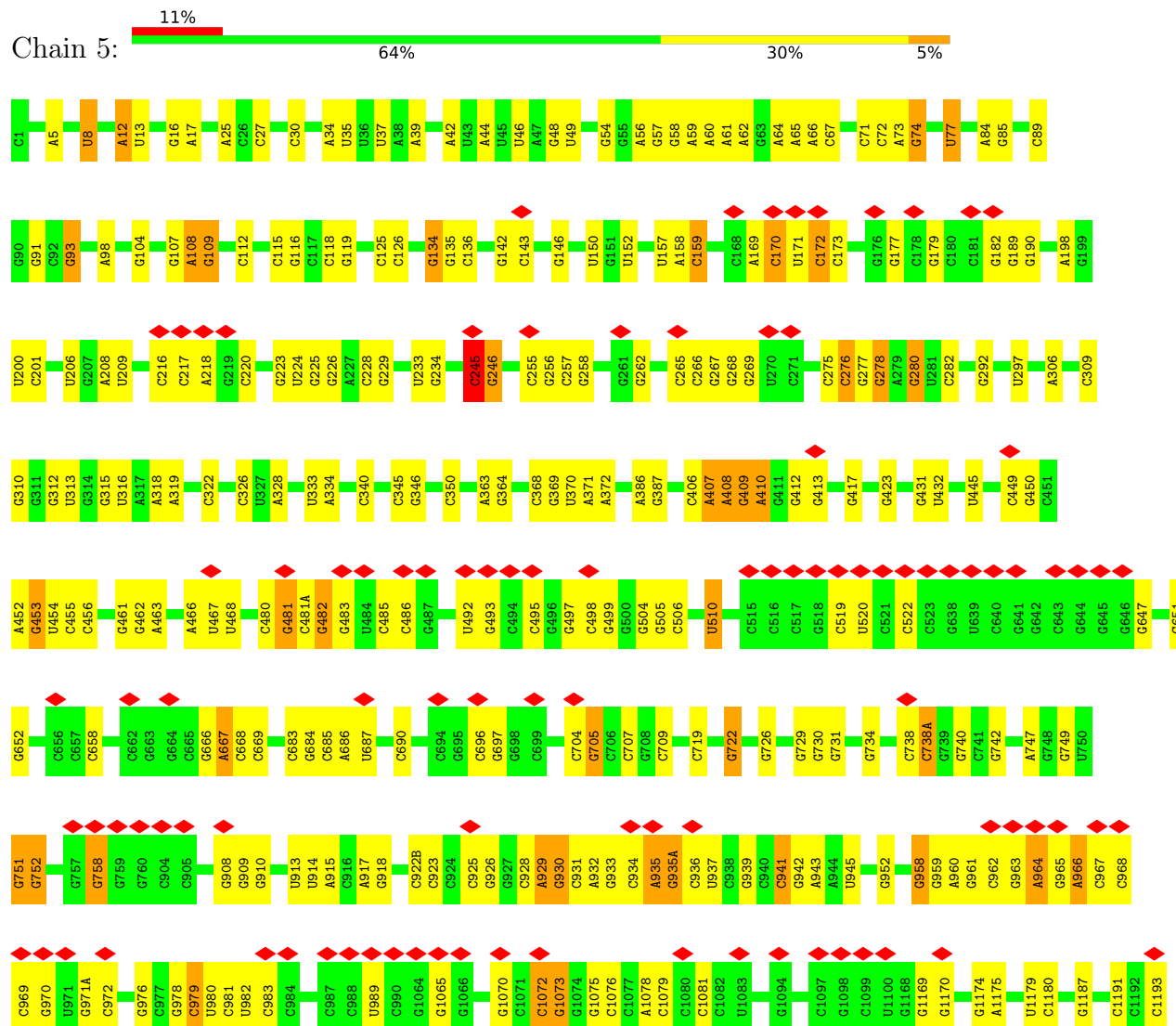
- Molecule 17: E-tRNA

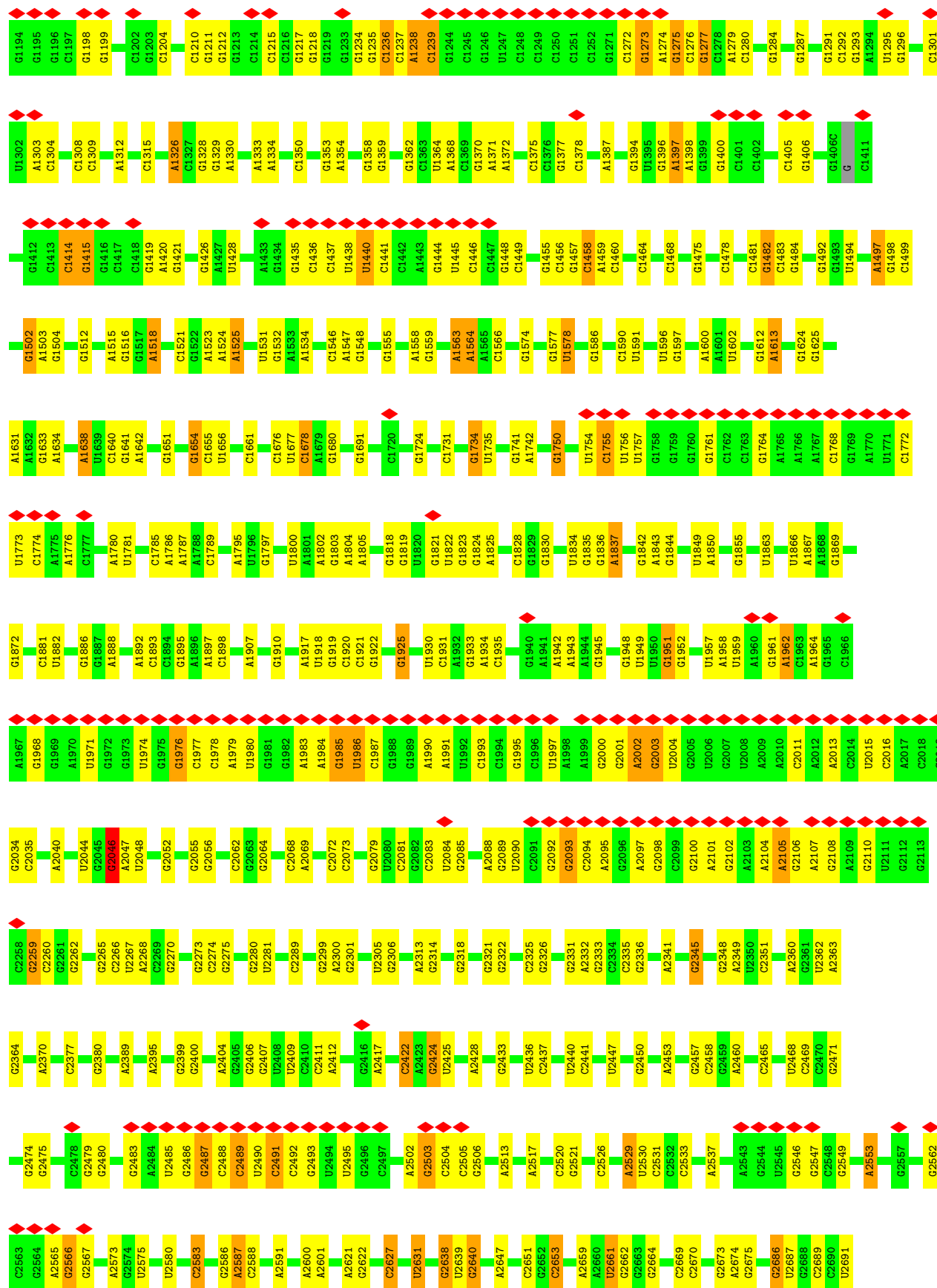


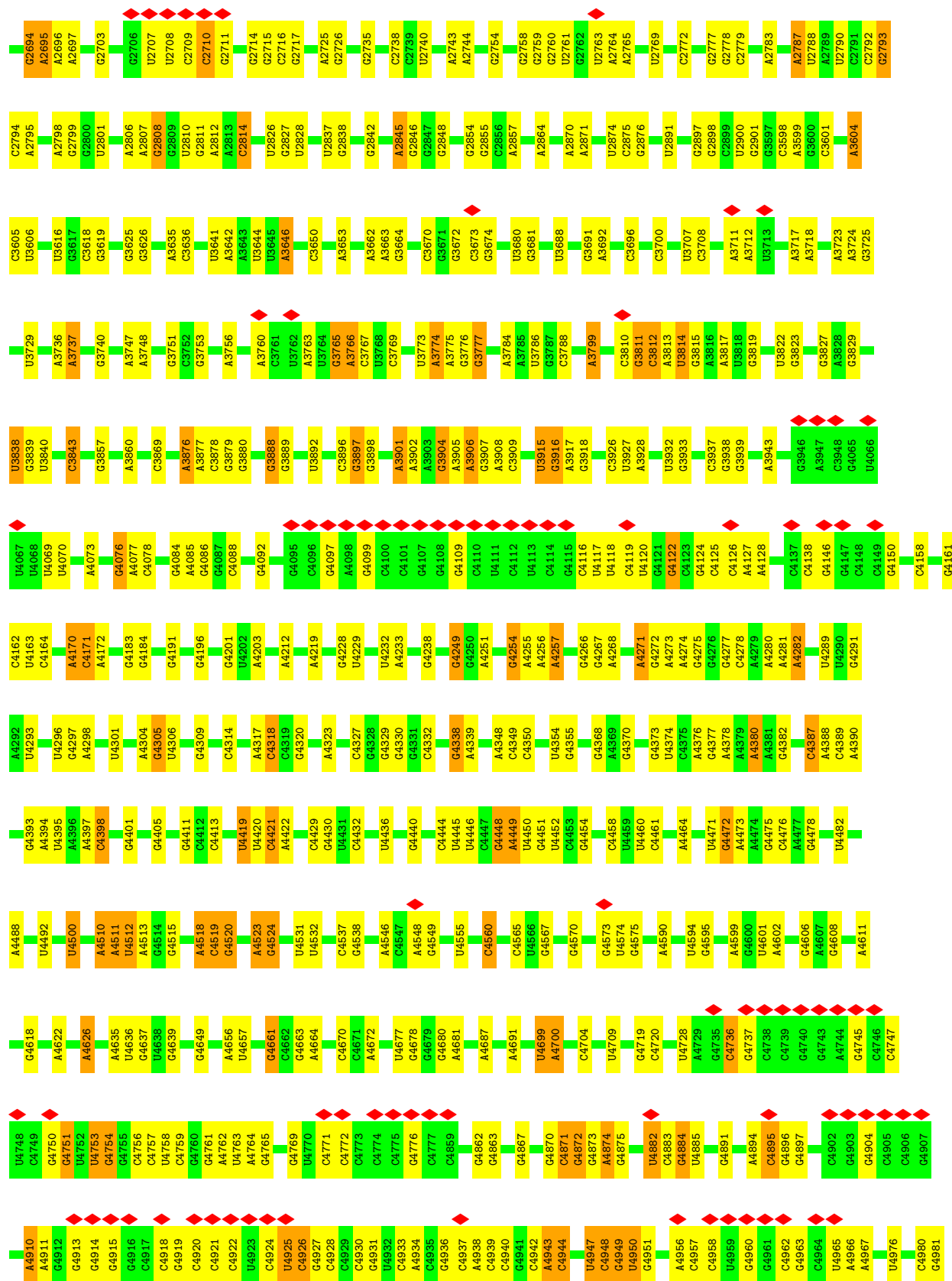
- Molecule 18: messenger RNA



- Molecule 19: 28S ribosomal RNA

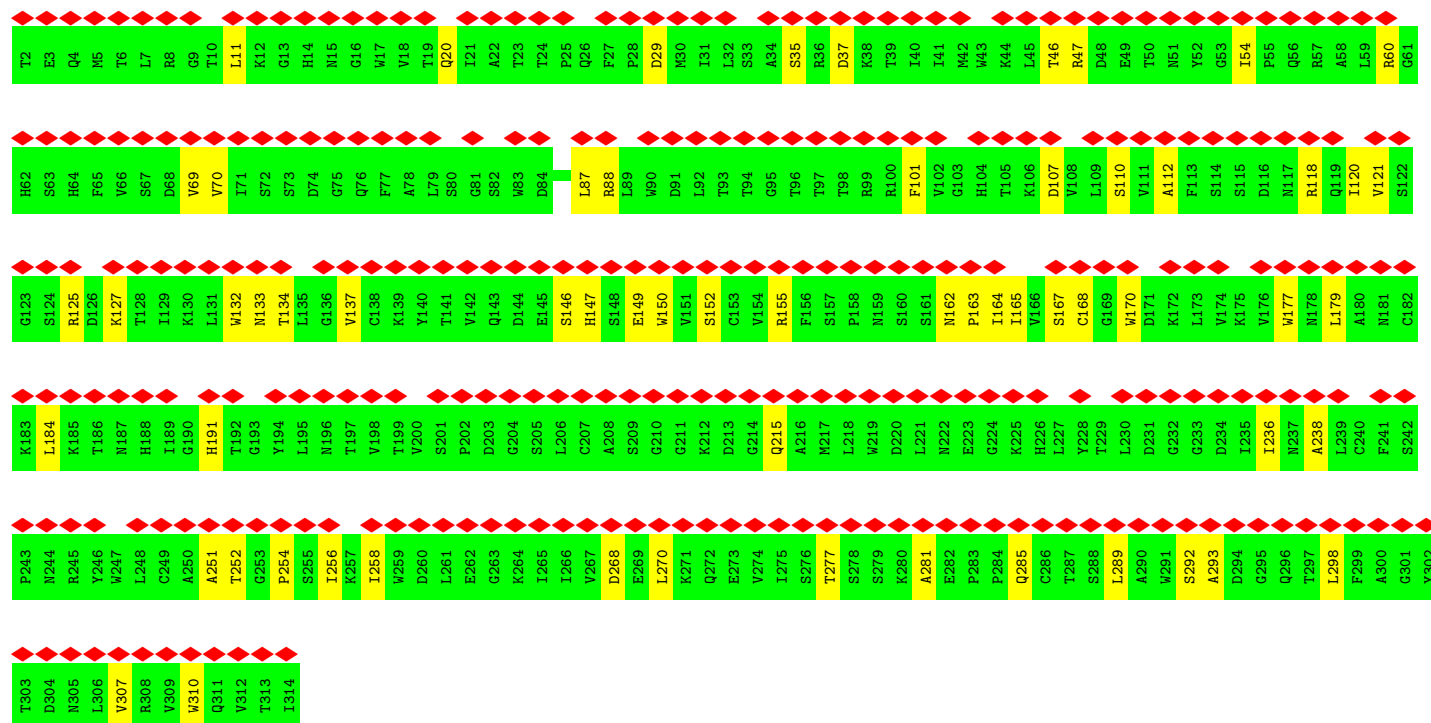
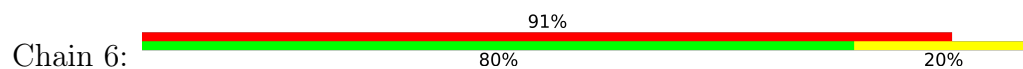




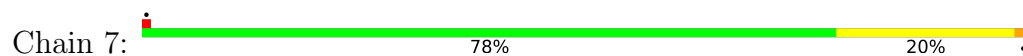




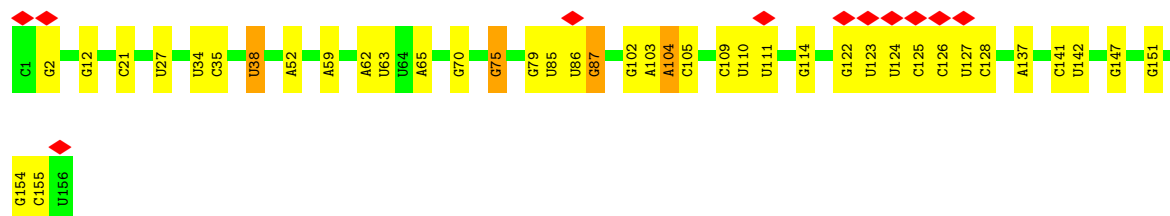
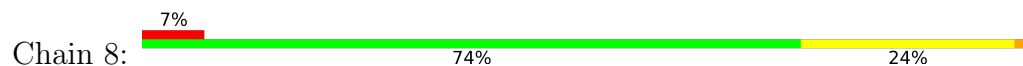
• Molecule 20: ribosomal protein RACK1



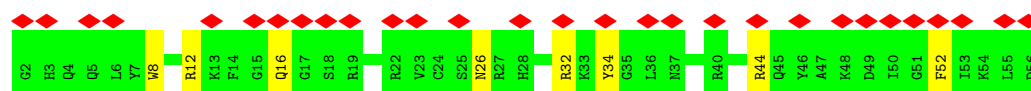
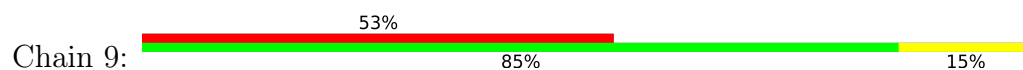
• Molecule 21: 5S ribosomal RNA



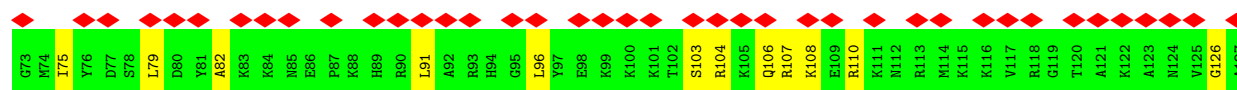
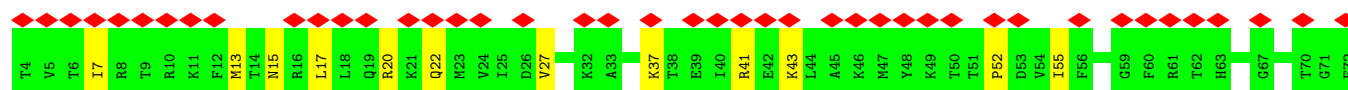
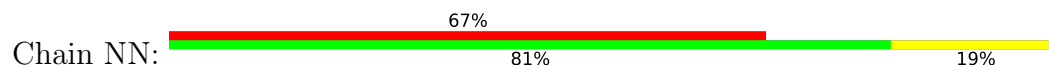
• Molecule 22: 5.8S ribosomal RNA



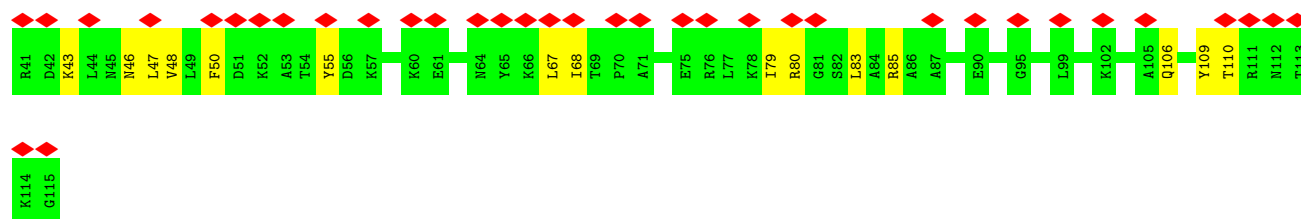
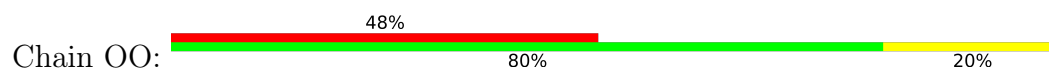
• Molecule 23: uS14



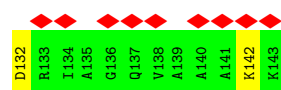
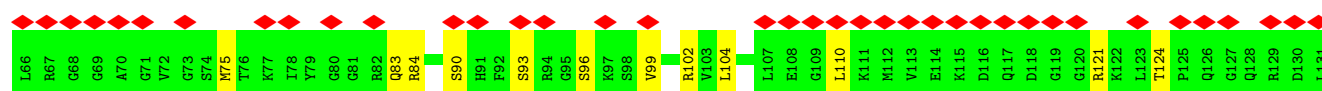
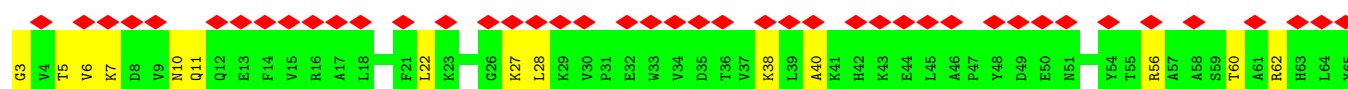
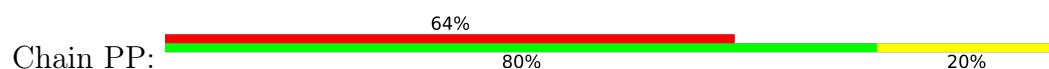
• Molecule 24: eS24



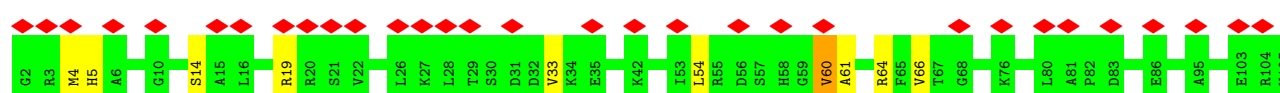
• Molecule 25: ribosomal protein eS25

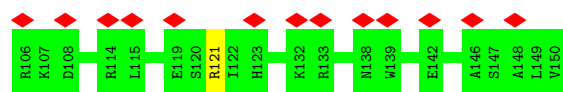


• Molecule 26: eS19

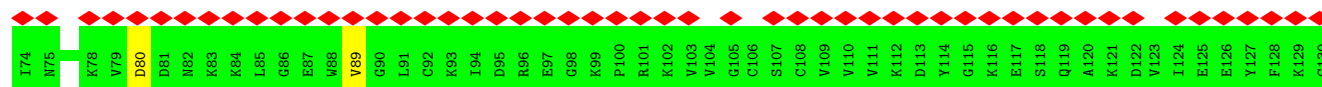
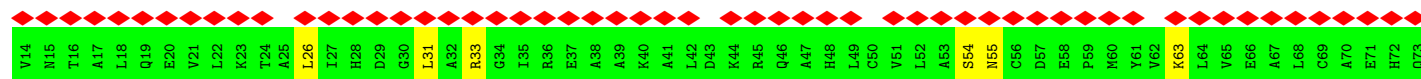


• Molecule 27: ribosomal protein uS15

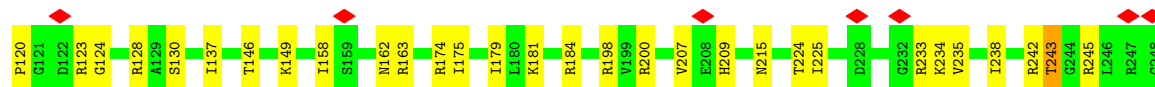
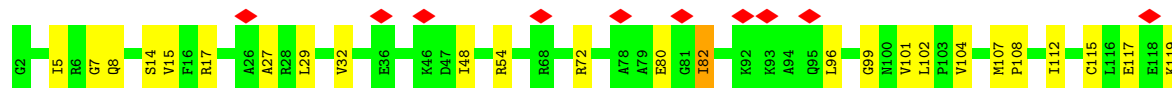
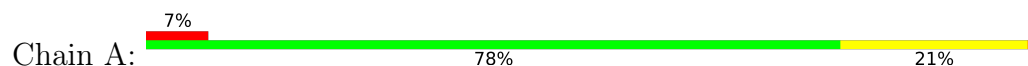




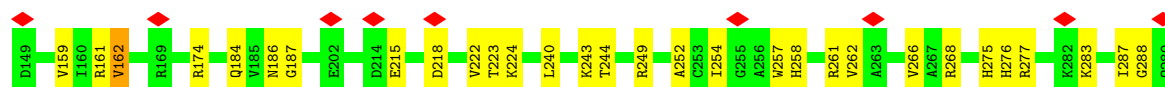
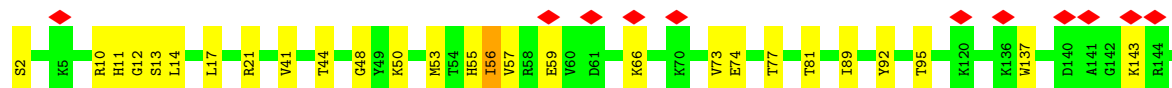
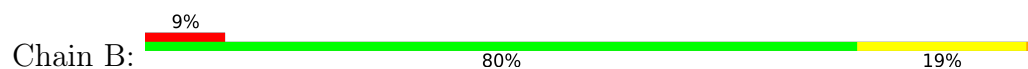
- Molecule 28: 40S ribosomal protein S12



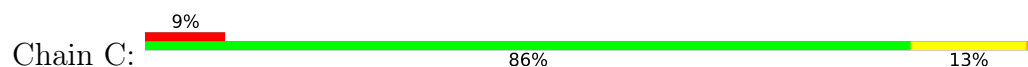
- Molecule 29: uL2

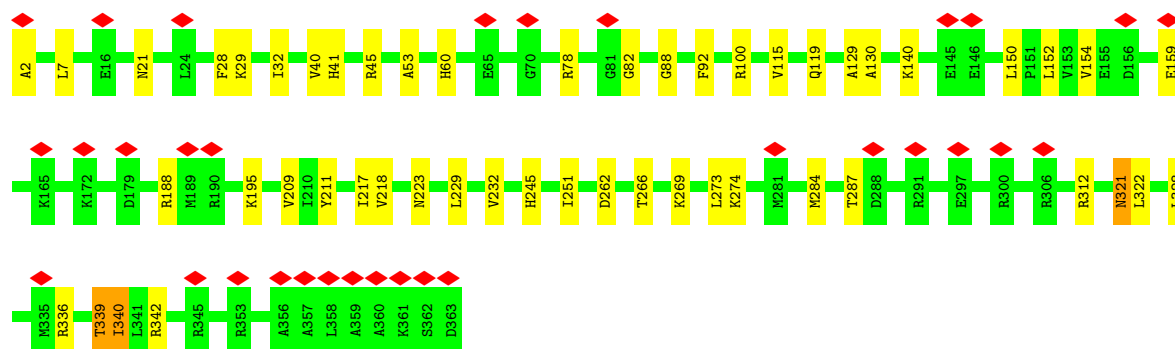


- Molecule 30: uL3

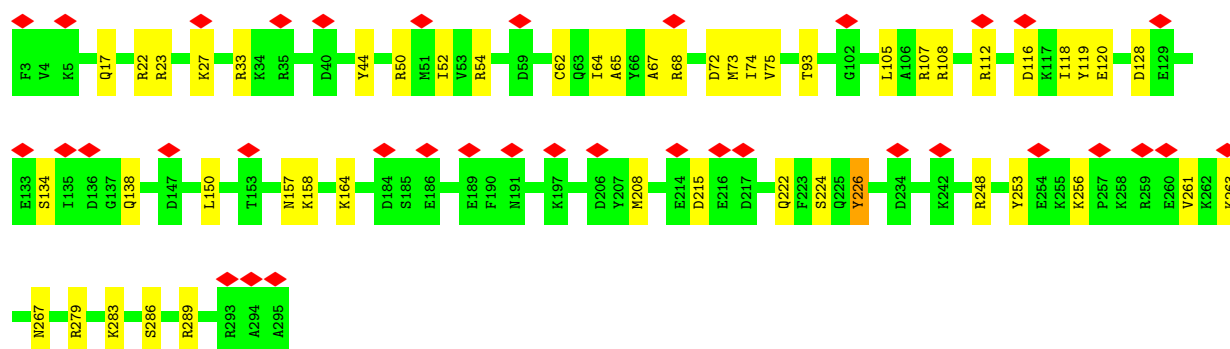
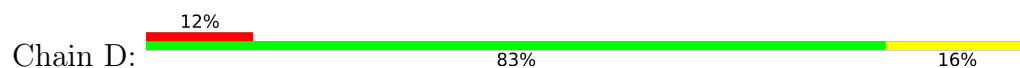


- Molecule 31: uL4

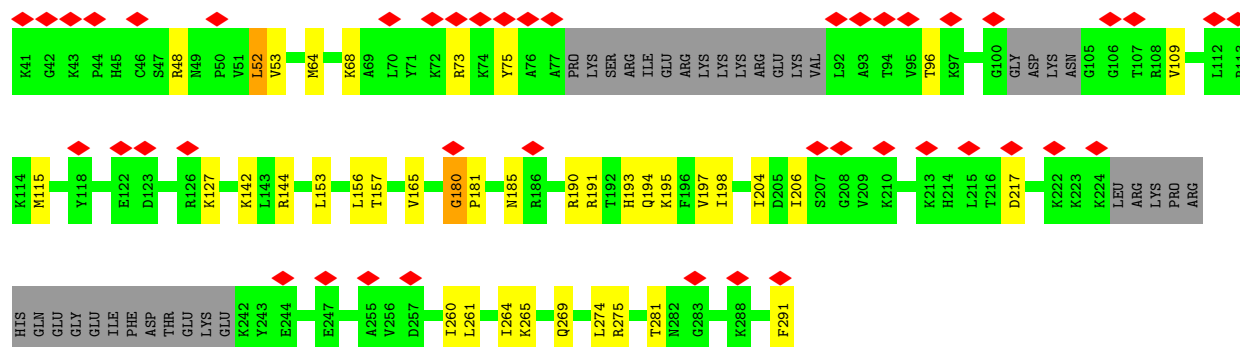




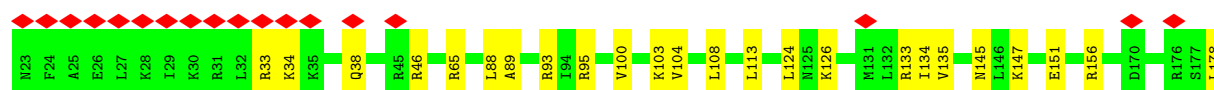
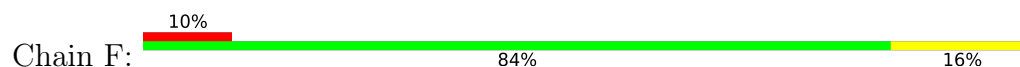
• Molecule 32: 60S ribosomal protein L5

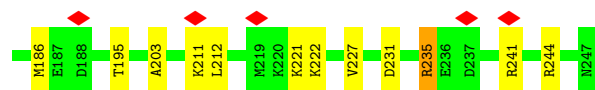


• Molecule 33: 60S ribosomal protein L6

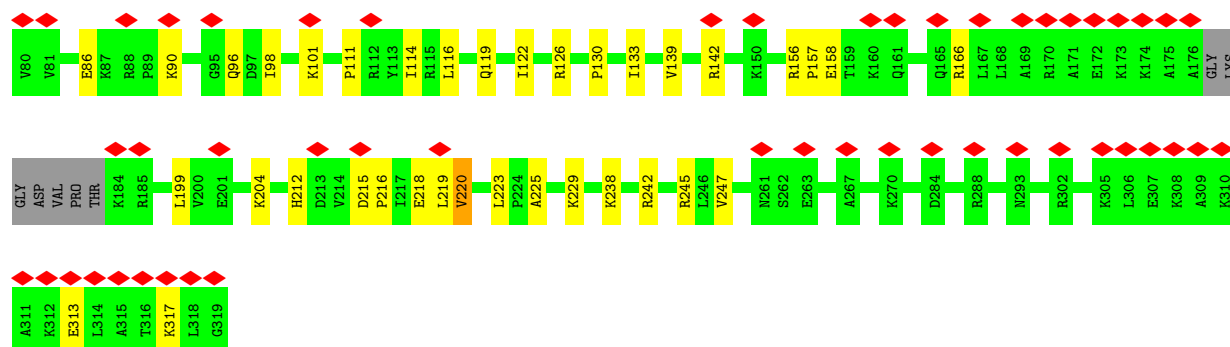
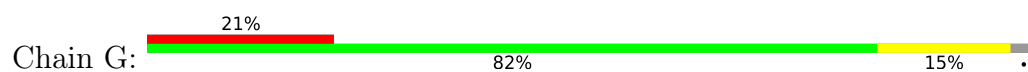


• Molecule 34: uL30

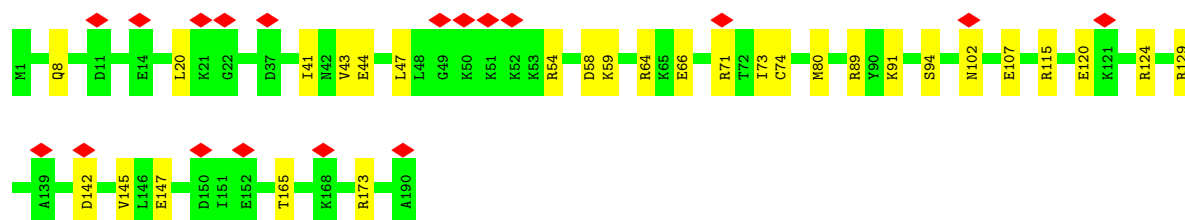
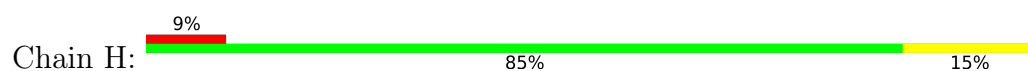




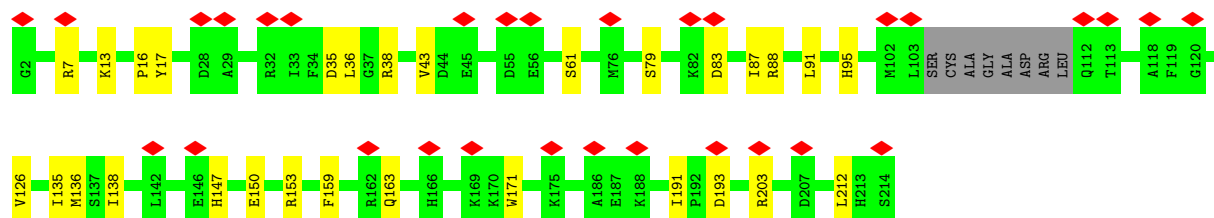
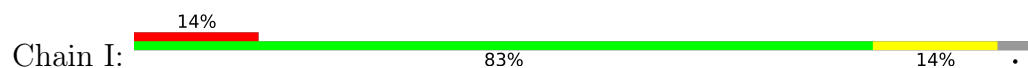
- Molecule 35: eL8



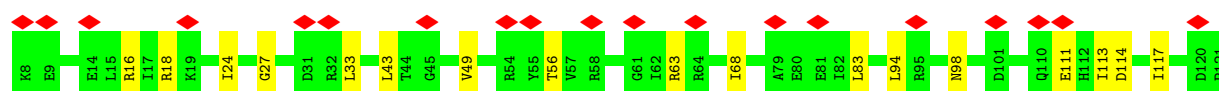
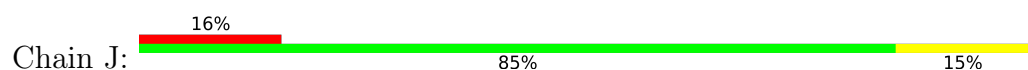
- Molecule 36: uL6

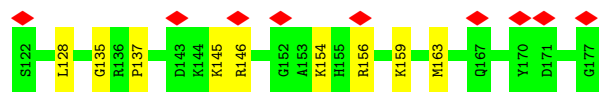


- Molecule 37: Ribosomal protein L10 (Predicted)

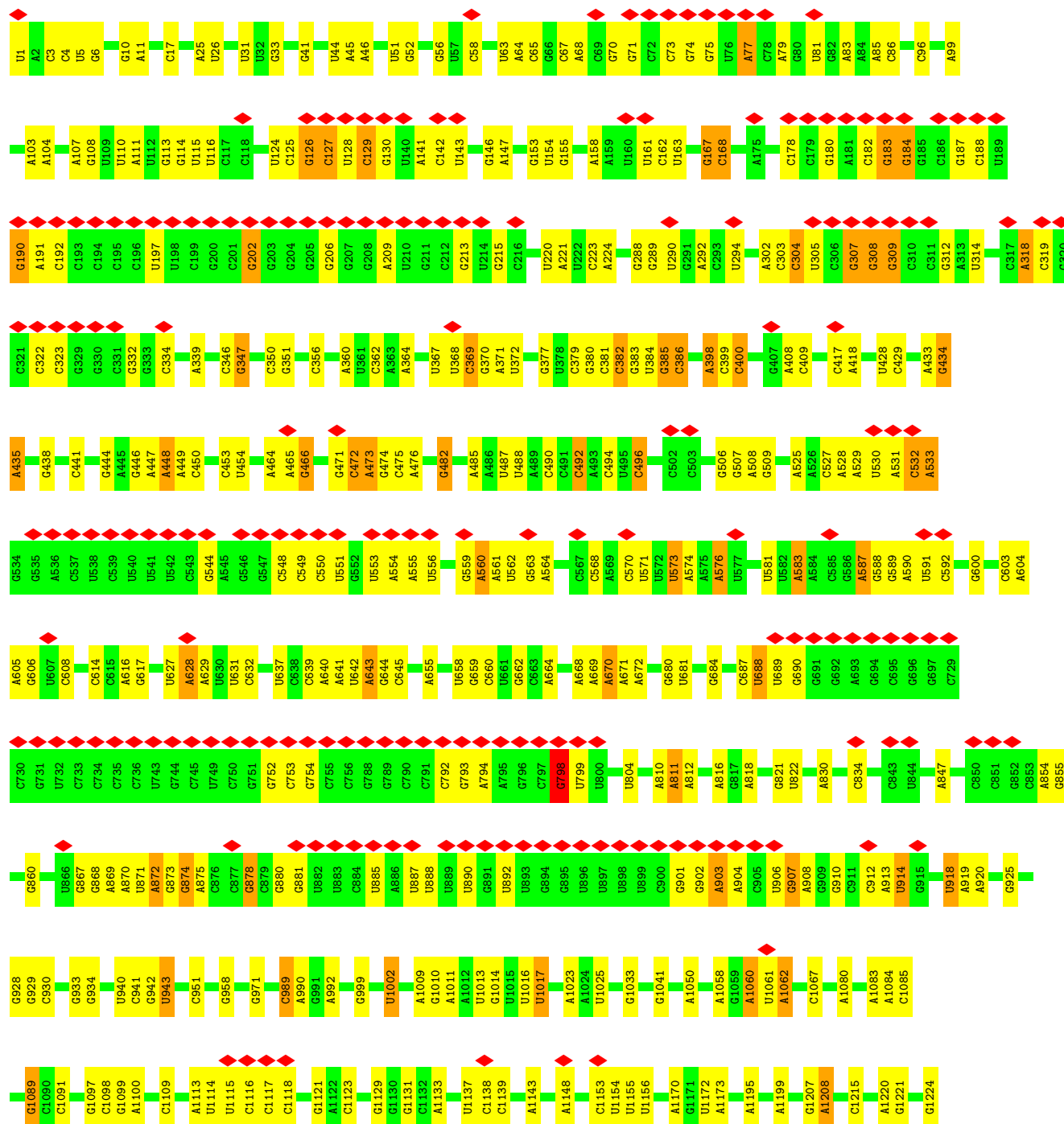


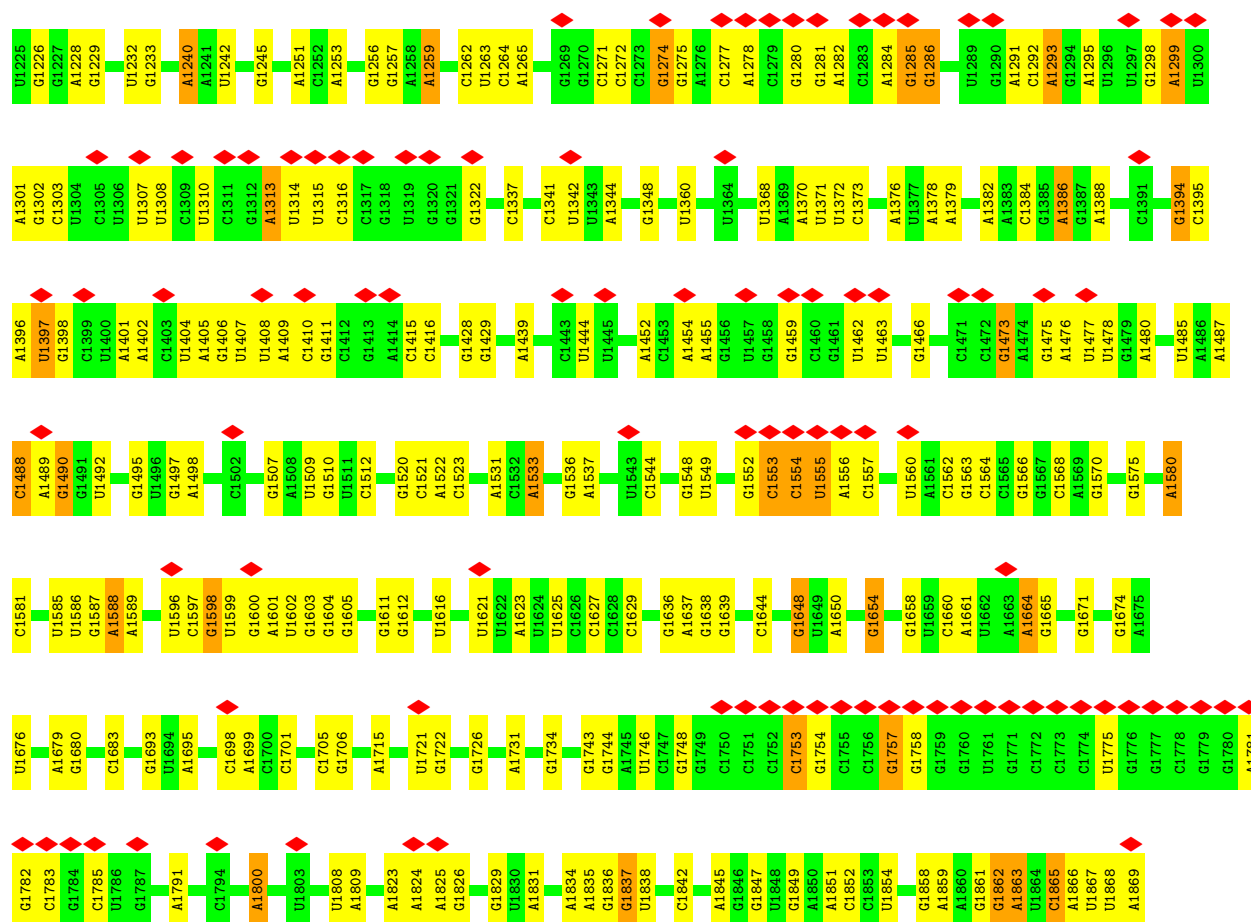
- Molecule 38: Ribosomal protein L11



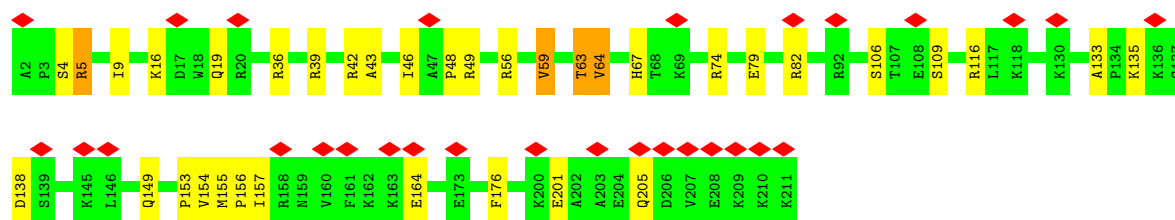
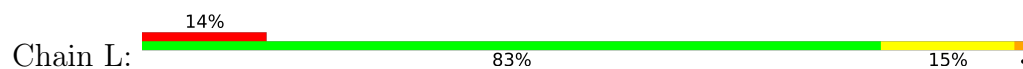


• Molecule 39: 18S ribosomal RNA

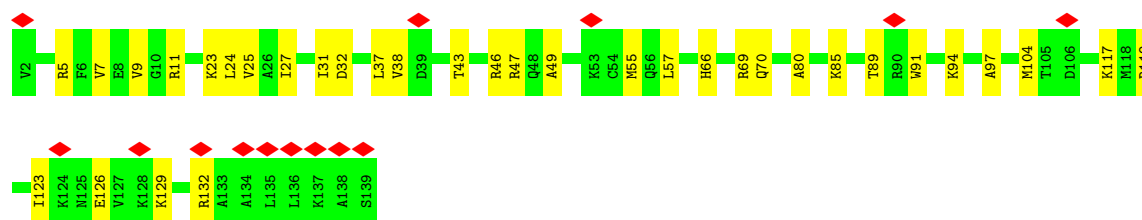
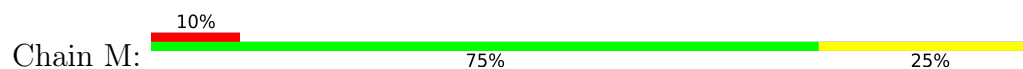




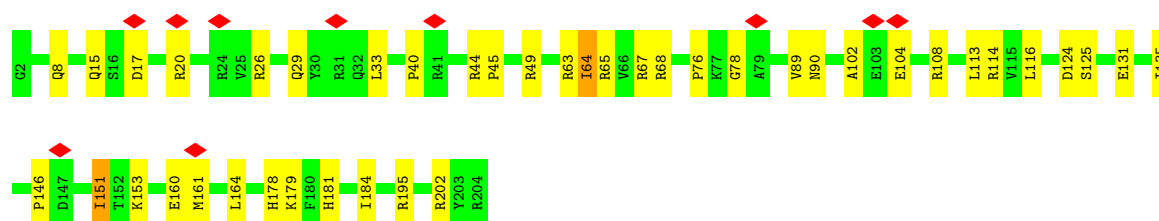
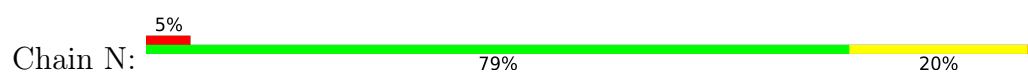
• Molecule 40: 60S ribosomal protein L13



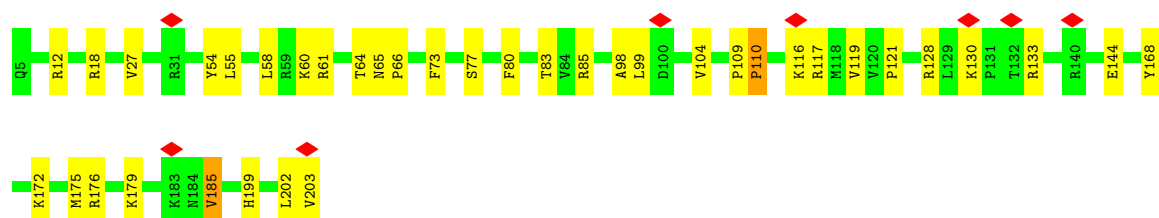
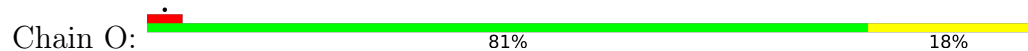
• Molecule 41: Ribosomal protein L14



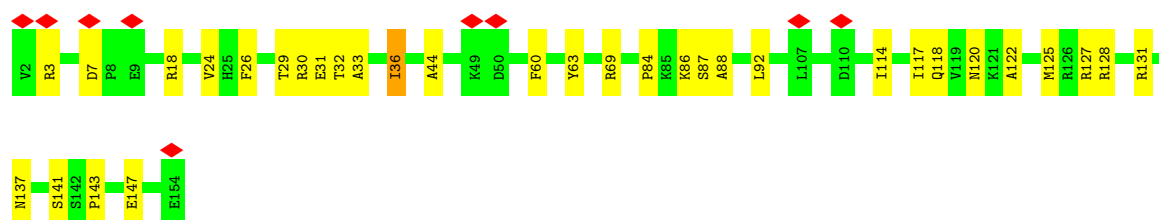
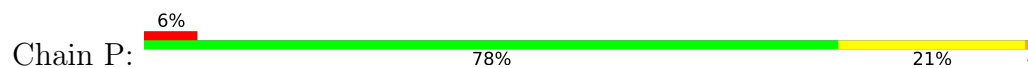
• Molecule 42: Ribosomal protein L15



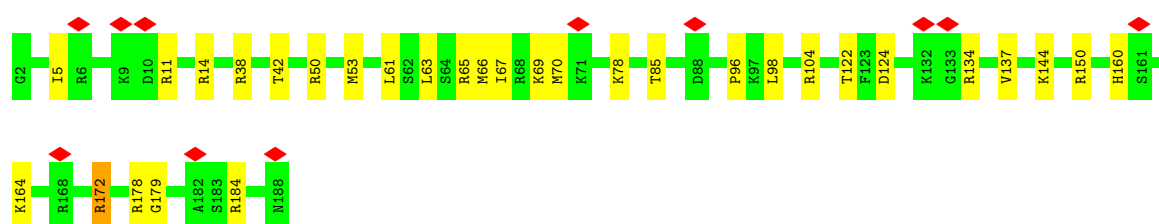
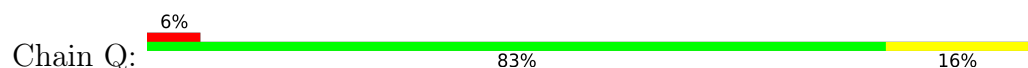
• Molecule 43: uL13



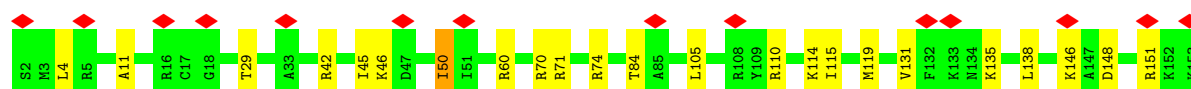
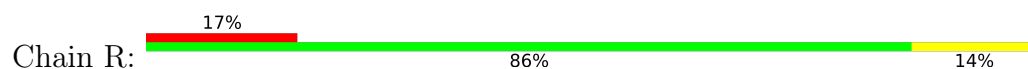
• Molecule 44: uL22

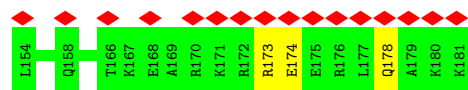


• Molecule 45: eL18

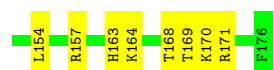
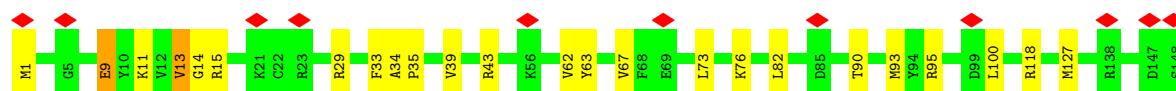
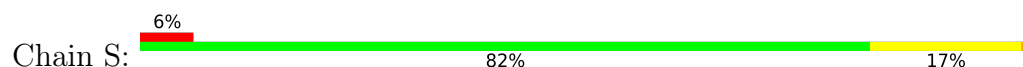


• Molecule 46: eL19

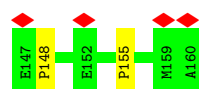
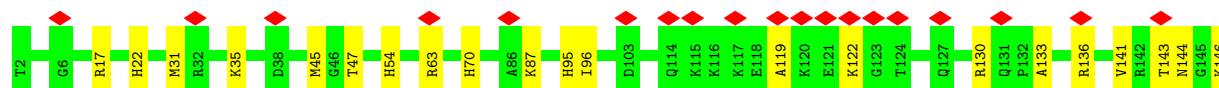
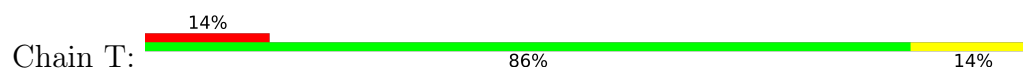




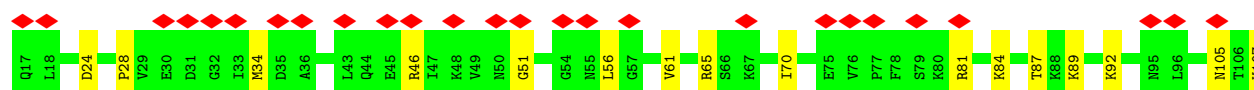
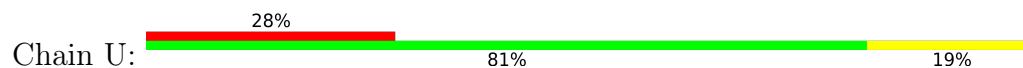
• Molecule 47: eL20



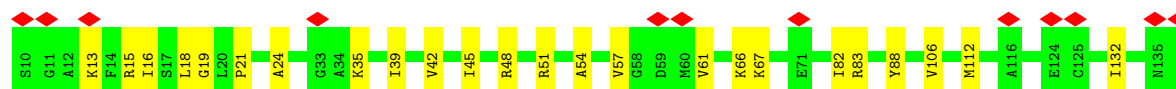
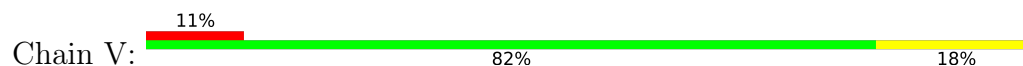
• Molecule 48: eL21



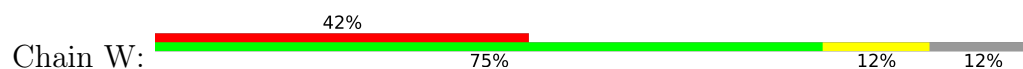
• Molecule 49: eL22

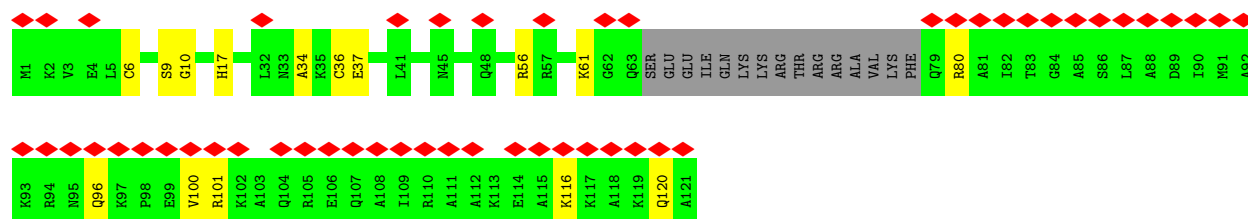


• Molecule 50: eL14

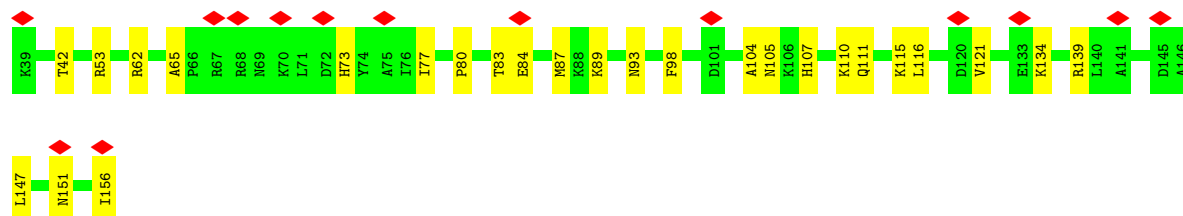
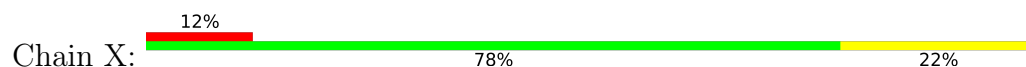


• Molecule 51: Ribosomal protein L24

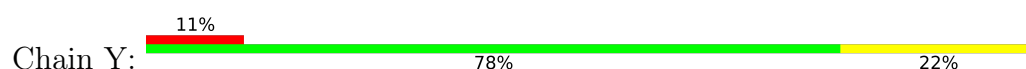




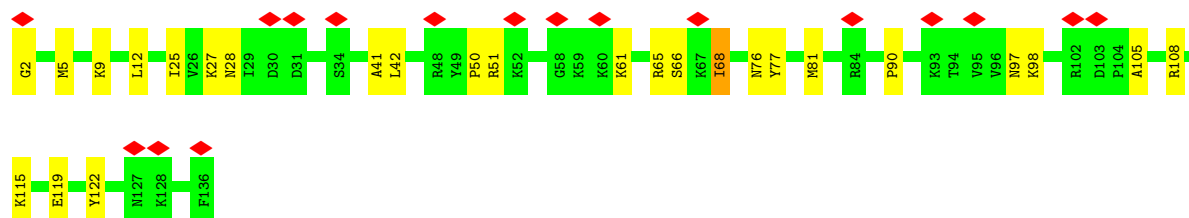
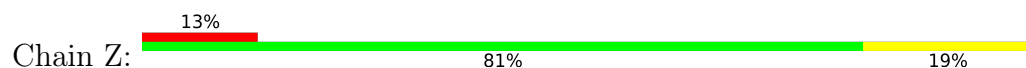
• Molecule 52: uL23



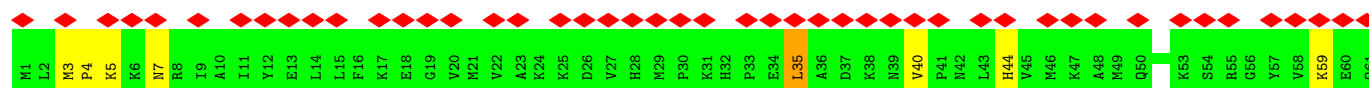
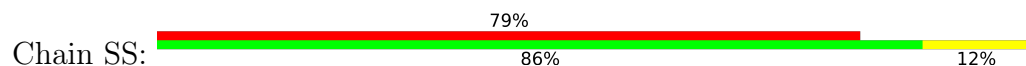
• Molecule 53: Ribosomal protein L26

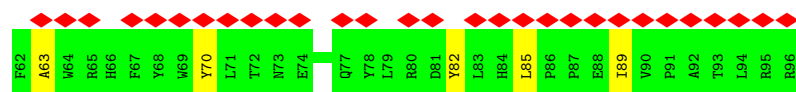


• Molecule 54: 60S ribosomal protein L27

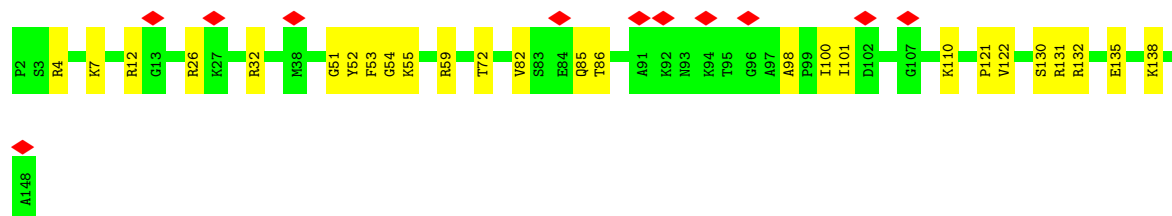
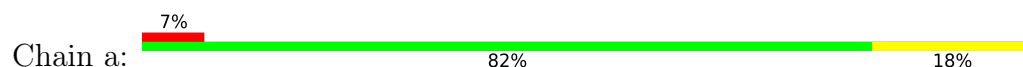


• Molecule 55: eS10

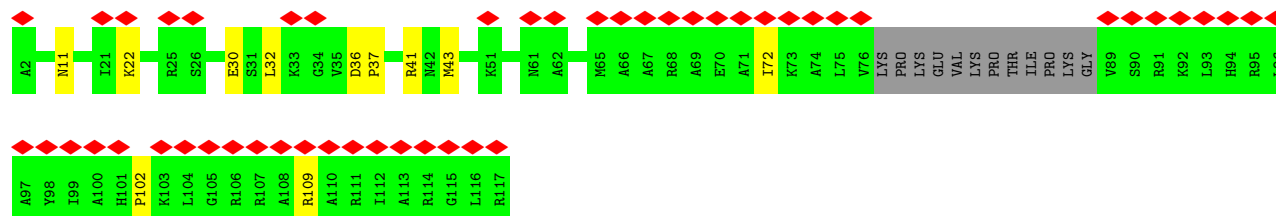
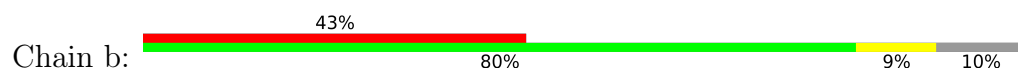




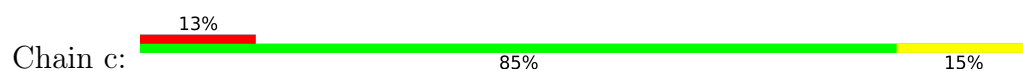
• Molecule 56: uL15



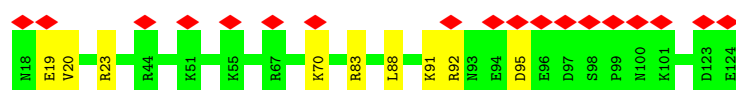
• Molecule 57: eL29



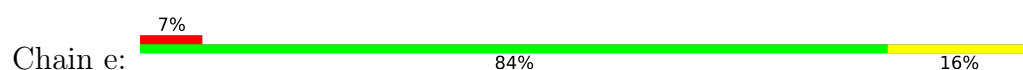
• Molecule 58: eL30



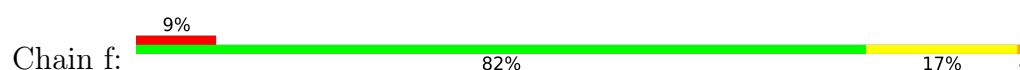
• Molecule 59: eL31



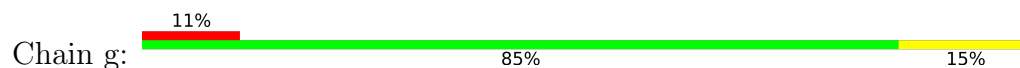
• Molecule 60: eL32



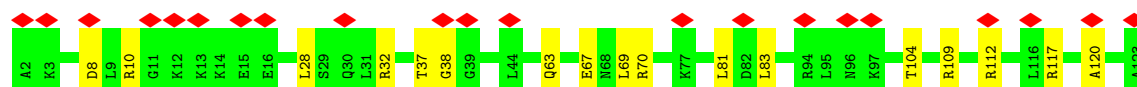
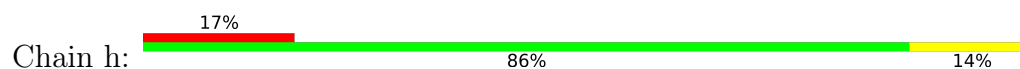
• Molecule 61: eL33



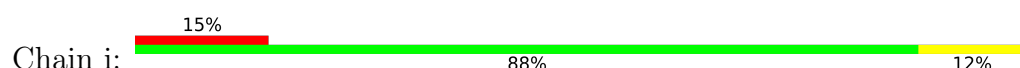
- Molecule 62: eL34



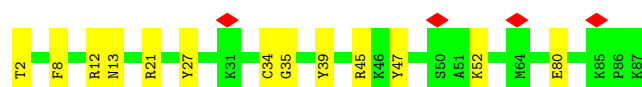
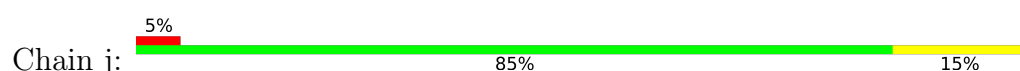
- Molecule 63: uL29



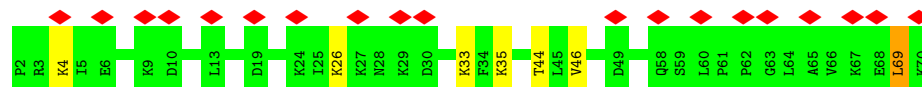
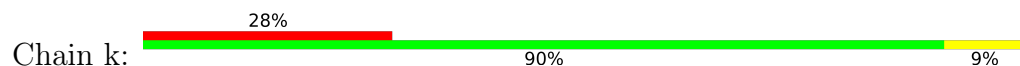
- Molecule 64: 60S ribosomal protein L36



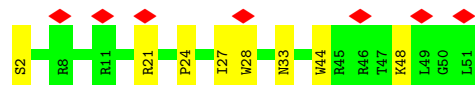
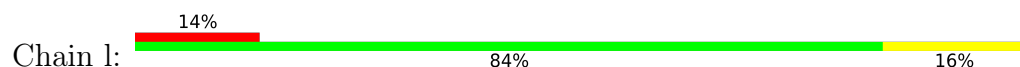
- Molecule 65: Ribosomal protein L37



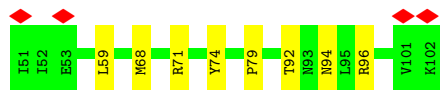
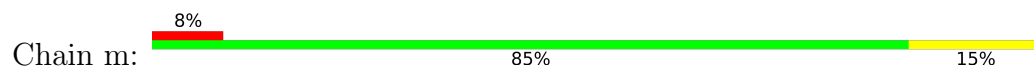
- Molecule 66: eL38



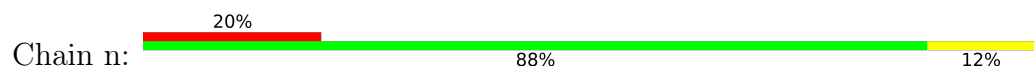
- Molecule 67: eL39



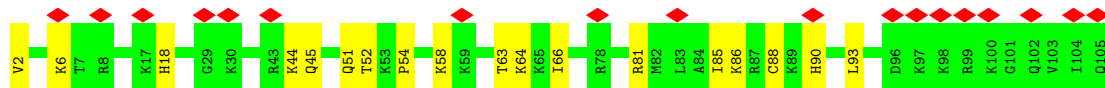
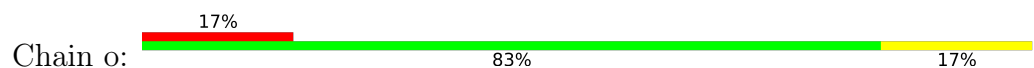
- Molecule 68: eL40



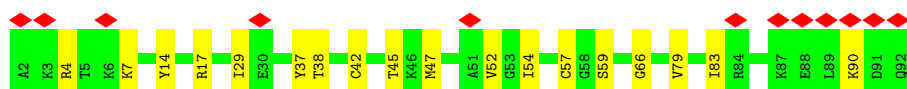
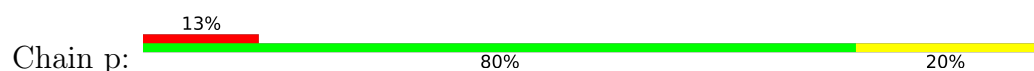
- Molecule 69: 60s ribosomal protein l41



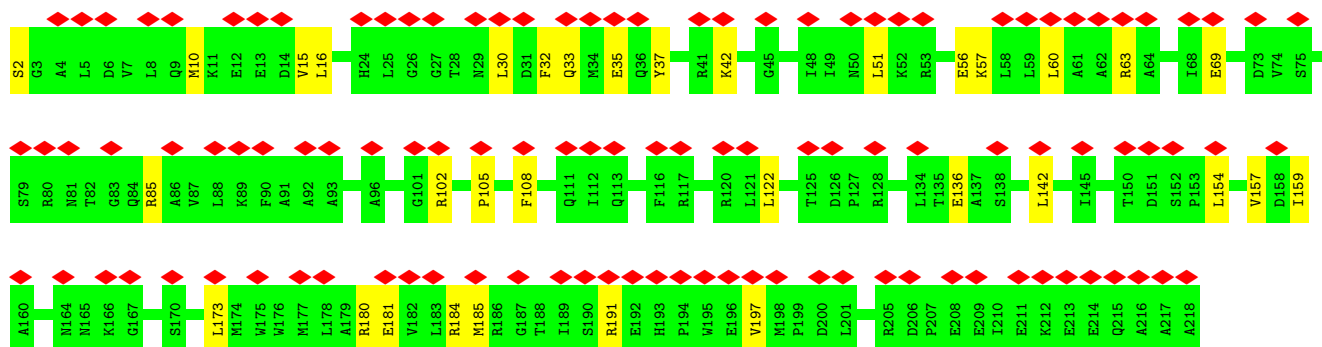
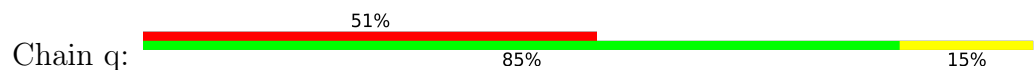
- Molecule 70: eL42



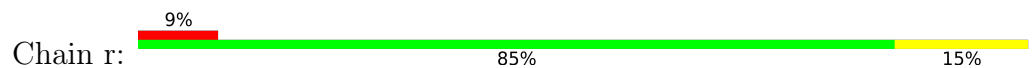
- Molecule 71: ribosomal protein eL43

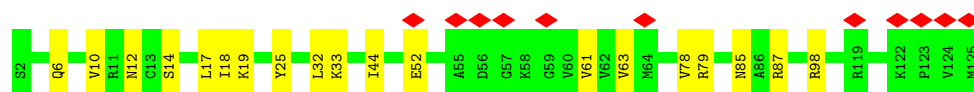


- Molecule 72: uS2

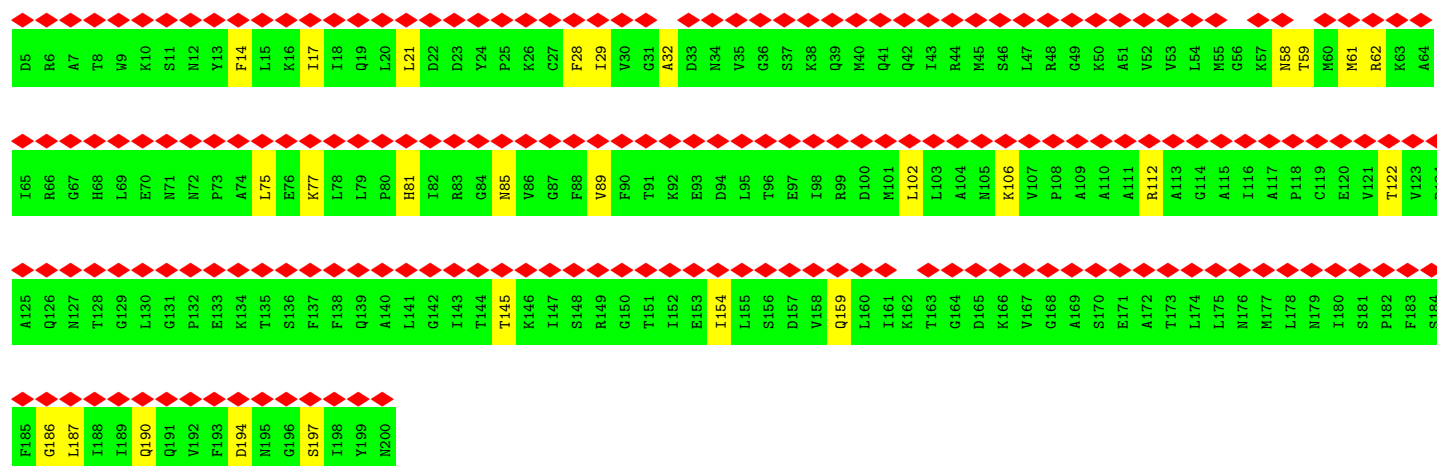
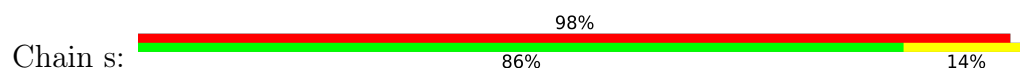


- Molecule 73: eL28

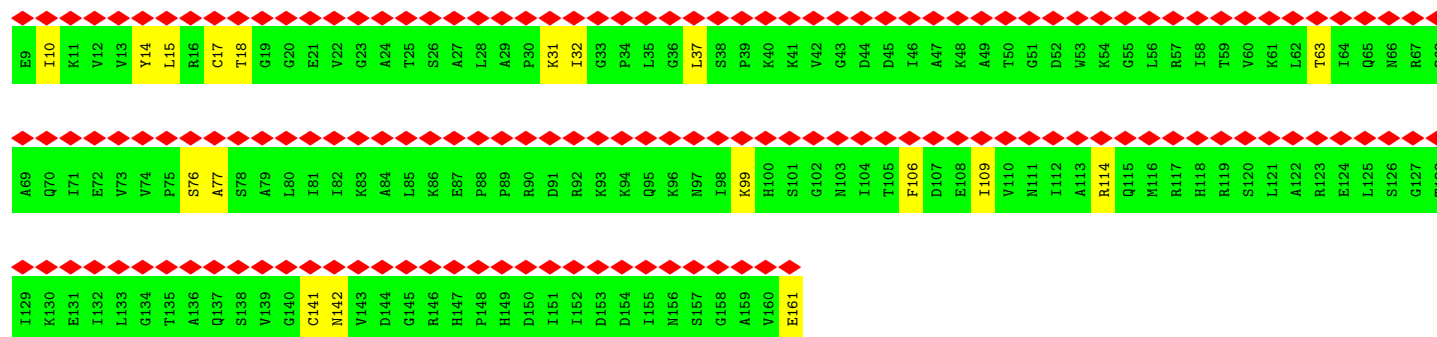
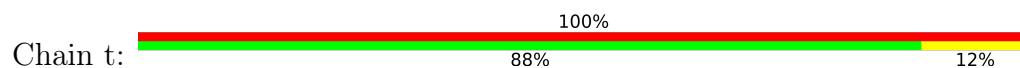




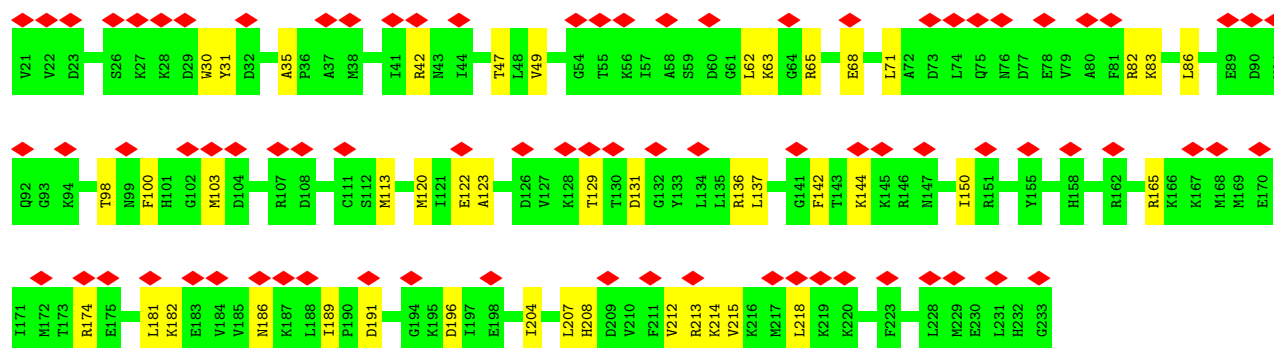
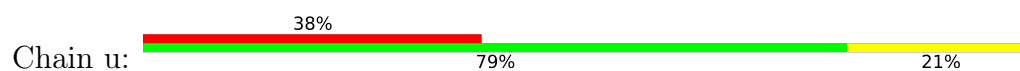
• Molecule 74: 60S acidic ribosomal protein P0



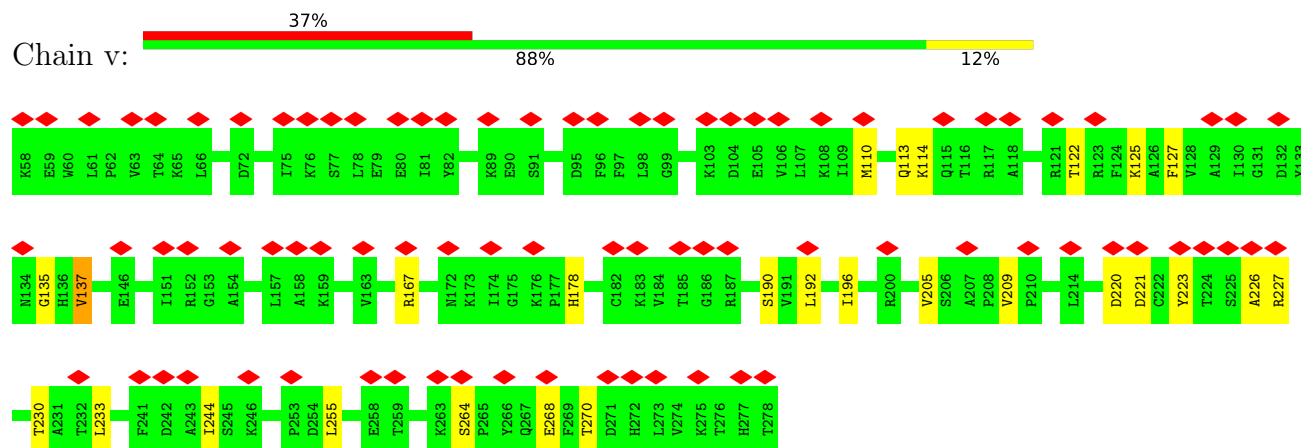
• Molecule 75: uL11



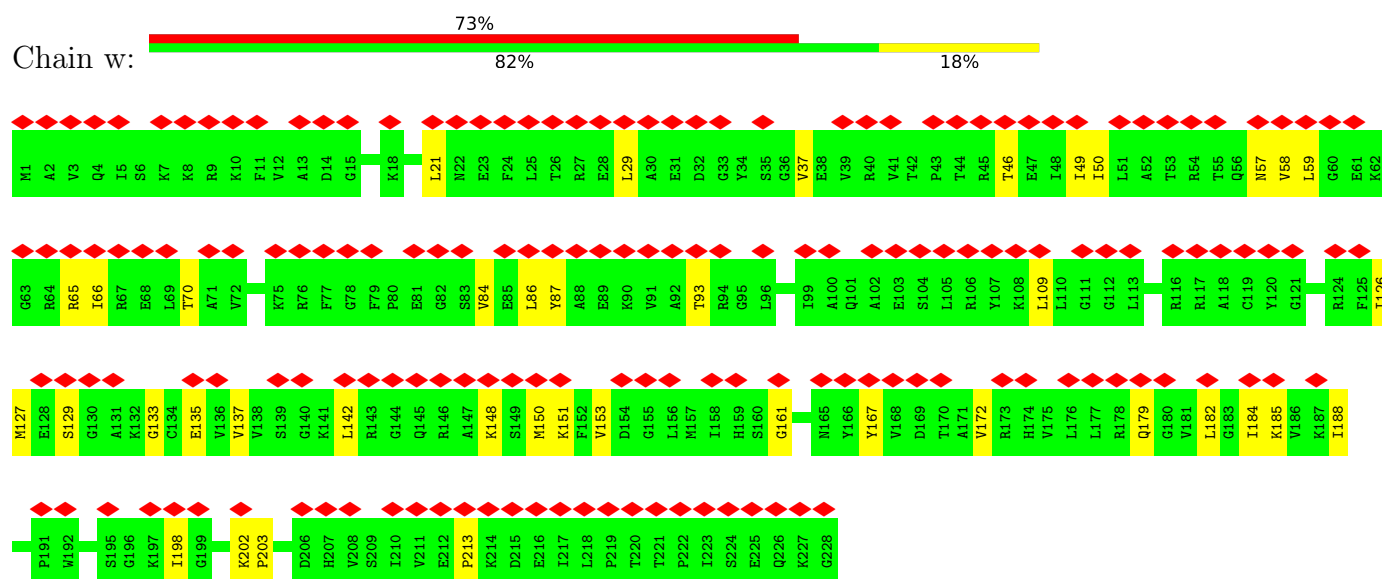
• Molecule 76: 40S ribosomal protein S3a



- Molecule 77: uS5

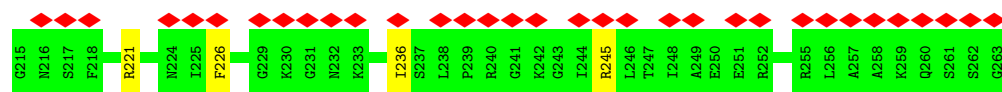


- Molecule 78: Ribosomal protein S3



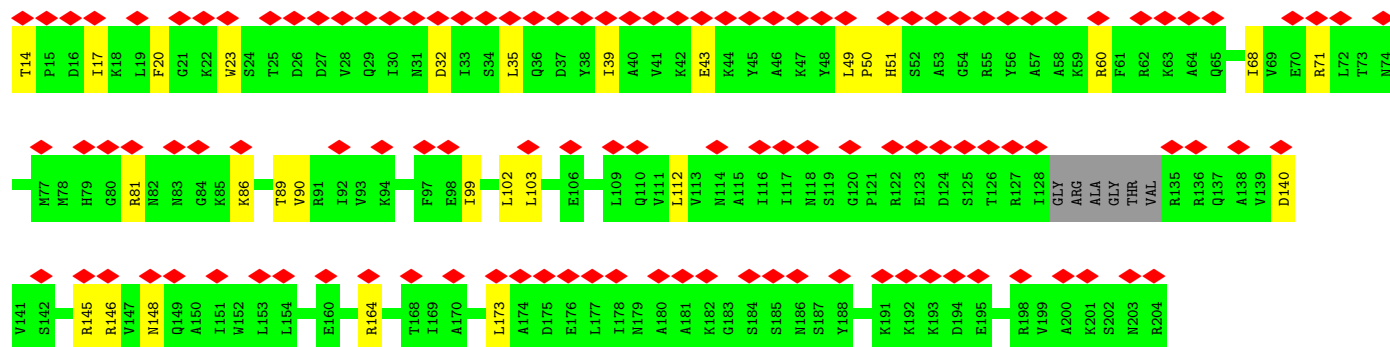
- Molecule 79: 40S ribosomal protein S4





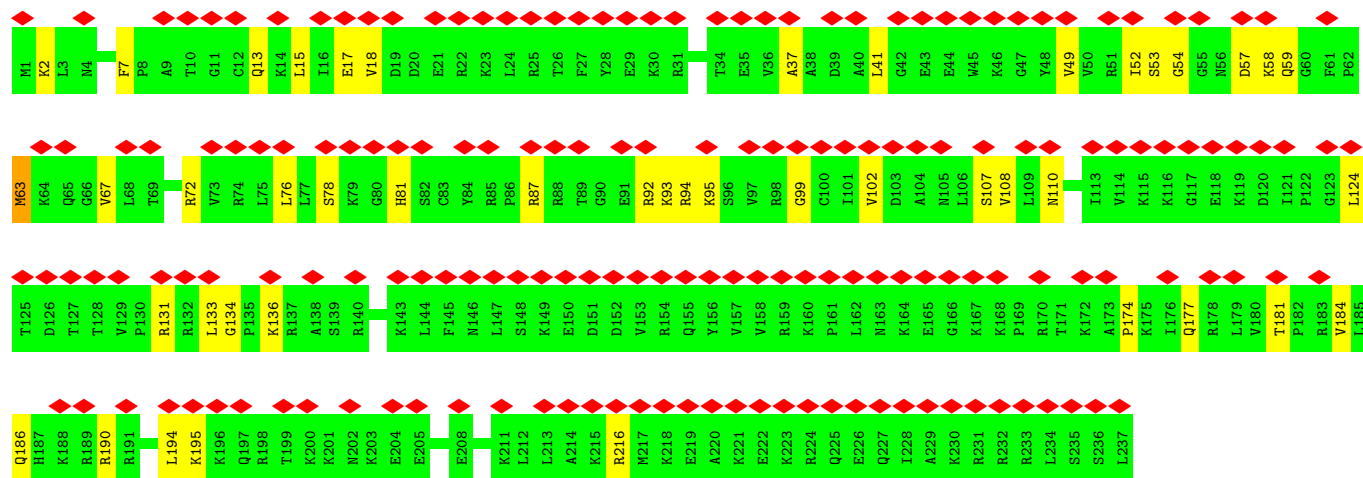
• Molecule 80: Ribosomal protein S5

Chain y:



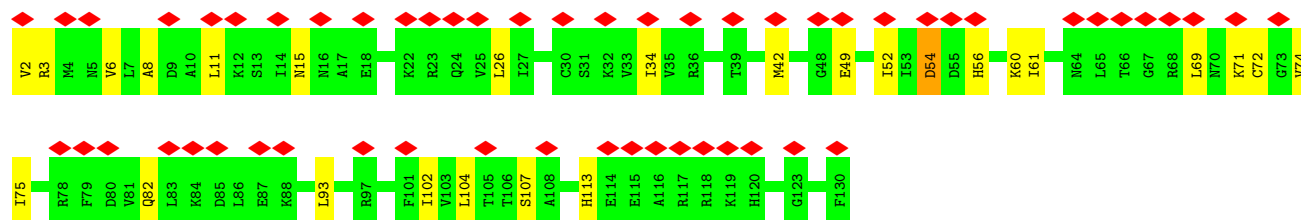
• Molecule 81: 40S ribosomal protein S6

Chain z:

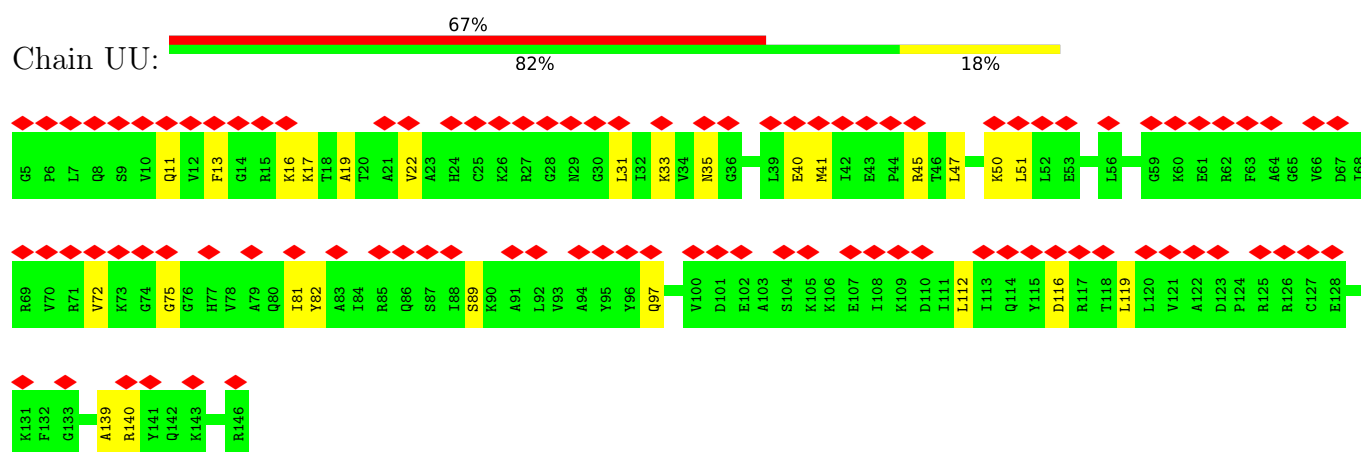


• Molecule 82: Ribosomal protein S15a

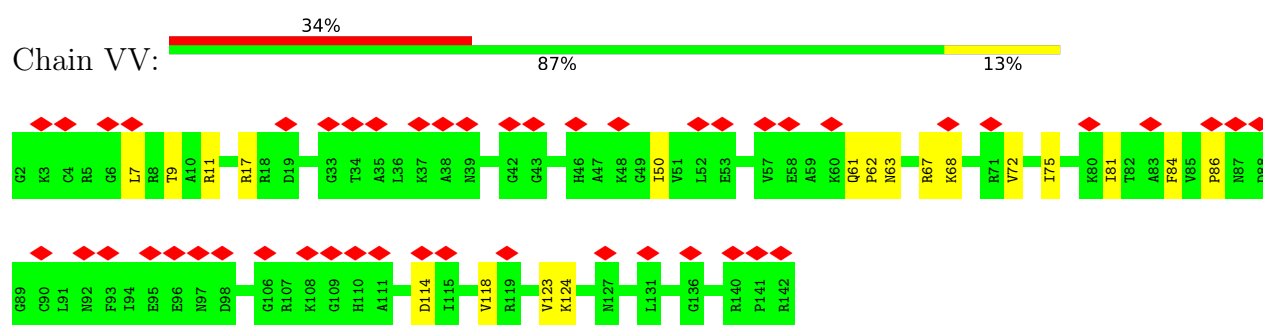
Chain TT:



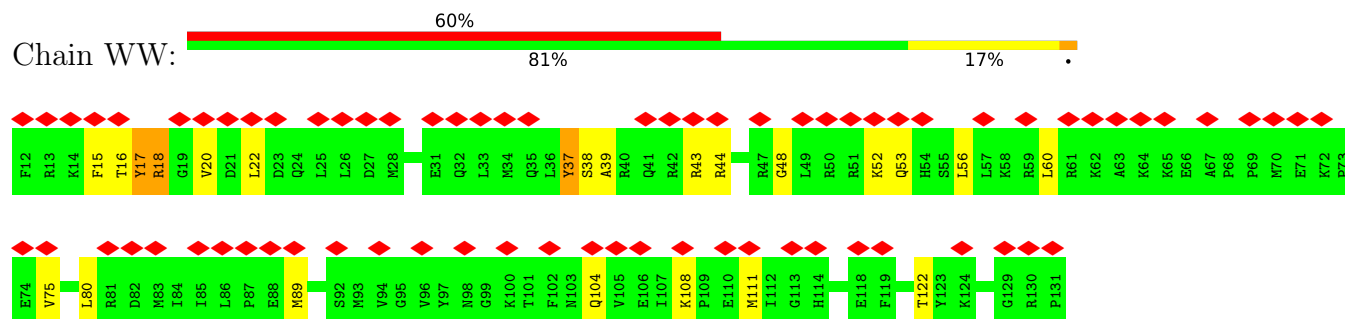
• Molecule 83: Ribosomal protein S16



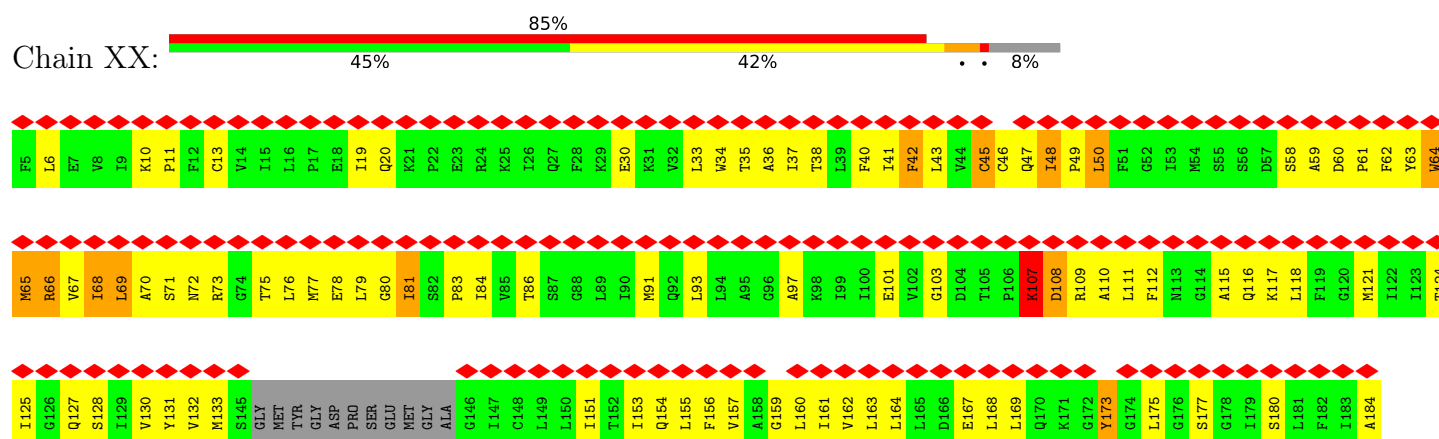
• Molecule 84: Ribosomal protein S23

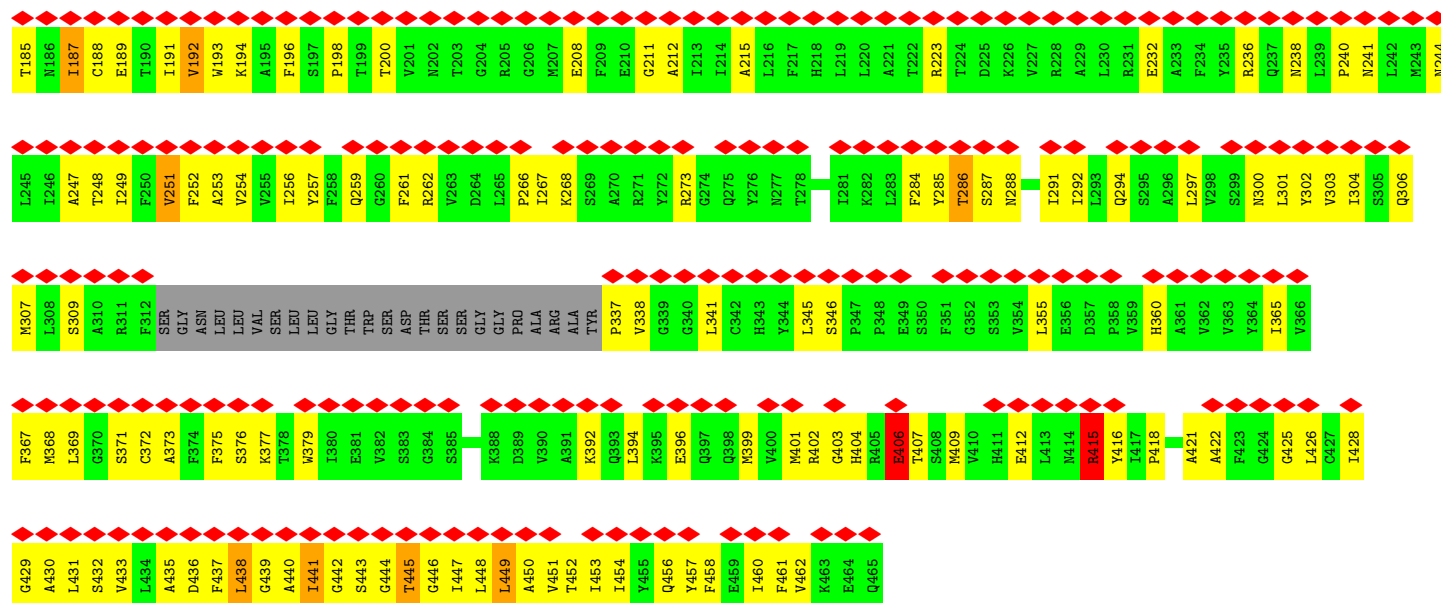


• Molecule 85: uS19

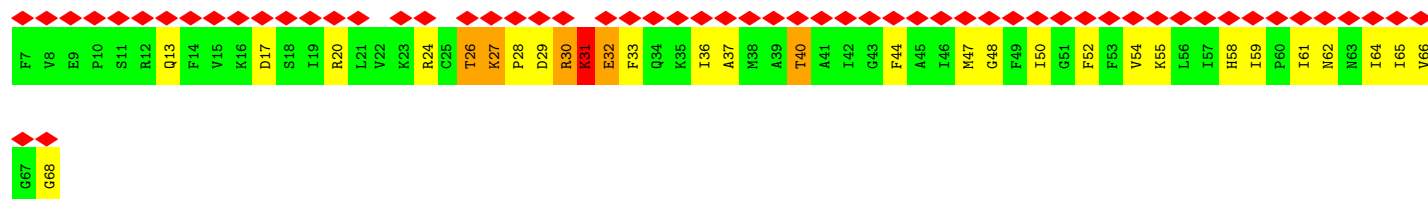


• Molecule 86: Protein transport protein Sec61 subunit alpha isoform 1

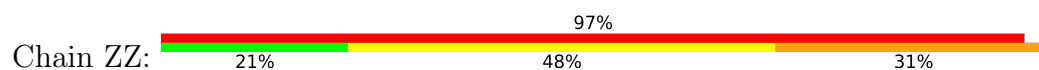




• Molecule 87: Protein transport protein Sec61 subunit gamma



• Molecule 88: Protein transport protein Sec61 subunit beta



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	12749	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	28	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.460	Depositor
Minimum map value	-0.305	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.020	Depositor
Recommended contour level	0.08	Depositor
Map size ($\text{\AA}$)	429.264, 429.264, 429.264	wwPDB
Map dimensions	396, 396, 396	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.084, 1.084, 1.084	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	AA	0.27	0/447	0.57	0/587
2	BB	0.29	0/1510	0.69	3/2022 (0.1%)
3	CC	0.38	0/1715	0.71	0/2287
4	DD	0.32	0/1550	0.64	1/2069 (0.0%)
5	EE	0.40	0/1195	0.66	0/1597
6	FF	0.30	0/490	0.61	0/656
7	GG	0.30	0/805	0.65	0/1081
8	HH	0.31	0/643	0.61	0/860
9	II	0.32	0/1208	0.69	0/1618
10	JJ	0.32	0/665	0.66	0/891
11	KK	0.26	0/1082	0.58	0/1452
12	LL	0.38	0/828	0.71	0/1109
13	MM	0.41	0/1029	0.72	0/1380
14	0	0.23	0/567	0.60	0/753
15	1	0.63	0/216	1.14	1/298 (0.3%)
16	2	0.47	2/1780 (0.1%)	0.62	0/2770
17	3	0.26	0/1783	0.43	0/2773
18	4	0.35	0/141	0.49	0/217
19	5	0.51	0/84978	0.54	12/132528 (0.0%)
20	6	0.24	0/2493	0.57	0/3394
21	7	0.49	0/2858	0.45	0/4455
22	8	0.51	0/3581	0.48	0/5577
23	9	0.31	0/470	0.62	0/623
24	NN	0.26	0/1028	0.62	0/1366
25	OO	0.29	0/604	0.59	0/810
26	PP	0.28	0/1115	0.64	0/1493
27	QQ	0.36	0/1226	0.59	0/1649
28	RR	0.25	0/918	0.64	0/1233
29	A	0.57	0/1936	0.84	1/2596 (0.0%)
30	B	0.53	0/3240	0.77	0/4339
31	C	0.52	0/2937	0.76	1/3946 (0.0%)
32	D	0.45	0/2437	0.71	0/3264

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	E	0.44	0/1762	0.73	0/2362
34	F	0.51	0/1911	0.72	0/2549
35	G	0.45	0/1910	0.71	0/2569
36	H	0.47	0/1535	0.75	2/2063 (0.1%)
37	I	0.48	0/1702	0.65	0/2272
38	J	0.42	0/1385	0.76	0/1852
39	K	0.36	0/40531	0.49	4/63162 (0.0%)
40	L	0.48	0/1733	0.73	0/2316
41	M	0.46	0/1158	0.76	0/1547
42	N	0.58	0/1746	0.77	0/2338
43	O	0.53	0/1662	0.75	2/2222 (0.1%)
44	P	0.53	0/1268	0.78	1/1700 (0.1%)
45	Q	0.55	0/1539	0.80	0/2054
46	R	0.47	0/1524	0.72	1/2013 (0.0%)
47	S	0.53	0/1501	0.72	0/2012
48	T	0.56	1/1326 (0.1%)	0.74	0/1770
49	U	0.36	0/823	0.64	0/1104
50	V	0.53	0/993	0.78	0/1332
51	W	0.43	0/873	0.63	0/1158
52	X	0.44	0/984	0.72	0/1323
53	Y	0.48	0/1132	0.69	0/1504
54	Z	0.46	0/1130	0.74	0/1507
55	SS	0.26	0/834	0.68	2/1125 (0.2%)
56	a	0.56	0/1191	0.79	0/1590
57	b	0.39	0/861	0.67	0/1138
58	c	0.43	0/771	0.66	0/1034
59	d	0.51	0/903	0.76	0/1216
60	e	0.54	0/1071	0.77	2/1429 (0.1%)
61	f	0.57	0/895	0.78	0/1198
62	g	0.49	0/916	0.77	0/1220
63	h	0.44	0/1021	0.65	0/1348
64	i	0.43	0/841	0.69	0/1112
65	j	0.53	0/720	0.78	0/952
66	k	0.39	0/575	0.61	0/761
67	l	0.49	0/459	0.71	0/608
68	m	0.51	0/435	0.67	0/575
69	n	0.53	0/240	0.83	0/305
70	o	0.49	0/864	0.70	0/1140
71	p	0.49	0/718	0.76	0/953
72	q	0.37	1/1747 (0.1%)	0.71	2/2374 (0.1%)
73	r	0.52	0/1010	0.78	0/1354
74	s	0.24	0/1530	0.56	0/2064
75	t	0.25	0/1174	0.66	0/1582

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
76	u	0.35	0/1756	0.64	0/2350
77	v	0.35	0/1753	0.68	1/2369 (0.0%)
78	w	0.28	0/1796	0.64	0/2417
79	x	0.32	0/2118	0.62	0/2849
80	y	0.31	0/1492	0.69	1/2005 (0.0%)
81	z	0.29	0/1946	0.62	0/2590
82	TT	0.37	0/1051	0.68	0/1406
83	UU	0.31	0/1146	0.66	0/1534
84	VV	0.37	0/1116	0.69	0/1490
85	WW	0.31	0/1017	0.67	0/1358
86	XX	0.91	1/3379 (0.0%)	1.01	12/4572 (0.3%)
87	YY	0.45	0/504	0.90	0/673
88	ZZ	0.52	0/236	1.50	5/321 (1.6%)
All	All	0.46	5/235689 (0.0%)	0.60	54/345434 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
8	HH	0	1
9	II	0	1
30	B	0	1
31	C	0	1
33	E	0	1
34	F	0	1
35	G	0	1
40	L	0	1
41	M	0	1
42	N	0	3
47	S	0	1
57	b	0	1
59	d	0	1
72	q	0	1
73	r	0	1
82	TT	0	1
84	VV	0	1
85	WW	0	2
86	XX	0	3
87	YY	0	1
All	All	0	25

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
86	XX	107	LYS	C-N	43.40	1.94	1.33
16	2	7	G	C1'-N9	-7.04	1.36	1.47
48	T	130	ARG	C-N	-5.97	1.25	1.33
72	q	197	VAL	C-N	-5.82	1.22	1.33
16	2	66	C	C1'-N1	5.73	1.57	1.48

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
86	XX	107	LYS	O-C-N	-18.30	98.25	122.59
31	C	340	ILE	N-CA-C	-11.70	102.37	111.62
88	ZZ	69	GLY	CA-C-N	11.44	134.14	119.84
88	ZZ	69	GLY	C-N-CA	11.44	134.14	119.84
72	q	197	VAL	CA-C-N	11.30	135.81	120.67
72	q	197	VAL	C-N-CA	11.30	135.81	120.67
86	XX	48	ILE	CA-C-N	10.08	130.01	120.03
86	XX	48	ILE	C-N-CA	10.08	130.01	120.03
86	XX	48	ILE	N-CA-C	9.28	119.16	108.96
88	ZZ	69	GLY	N-CA-C	-8.99	103.80	115.22
2	BB	65	PRO	CA-C-N	8.34	125.49	120.24
2	BB	65	PRO	C-N-CA	8.34	125.49	120.24
44	P	36	ILE	N-CA-CB	-7.97	103.07	112.39
39	K	902	G	C4'-C3'-O3'	7.90	124.85	113.00
86	XX	415	ARG	O-C-N	-7.54	111.07	122.08
86	XX	81	ILE	N-CA-C	-7.42	105.31	112.29
77	v	135	GLY	N-CA-C	7.05	122.05	113.79
86	XX	69	LEU	CA-C-N	-7.02	112.12	122.86
86	XX	69	LEU	C-N-CA	-7.02	112.12	122.86
19	5	3876	A	C2'-C3'-O3'	6.60	119.40	109.50
86	XX	449	LEU	CA-CB-CG	-6.19	94.64	116.30
19	5	4446	U	C4'-C3'-O3'	-6.18	103.73	113.00
55	SS	63	ALA	CA-C-N	6.17	133.33	121.54
55	SS	63	ALA	C-N-CA	6.17	133.33	121.54
19	5	4170	A	C2'-C3'-O3'	6.15	118.73	109.50
19	5	245	C	C2'-C3'-O3'	6.07	118.60	109.50
88	ZZ	69	GLY	O-C-N	6.01	123.23	121.07
60	e	43	ASN	CA-C-N	5.94	128.24	120.28
60	e	43	ASN	C-N-CA	5.94	128.24	120.28
80	y	43	GLU	N-CA-CB	-5.93	107.41	114.17
4	DD	86	VAL	N-CA-C	-5.77	107.19	112.96
46	R	131	VAL	N-CA-C	-5.73	107.26	111.90
15	1	247	CYS	N-CA-C	5.68	122.91	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	5	3888	G	C2'-C3'-O3'	5.67	122.20	113.70
88	ZZ	83	SER	N-CA-C	-5.66	105.11	111.28
43	O	185	VAL	N-CA-CB	-5.64	102.60	112.08
36	H	107	GLU	CA-C-N	5.55	130.28	122.46
36	H	107	GLU	C-N-CA	5.55	130.28	122.46
86	XX	63	TYR	N-CA-C	5.48	117.06	111.14
19	5	1236	C	C4'-C3'-O3'	5.46	121.19	113.00
19	5	2046	G	P-O3'-C3'	5.46	128.38	120.20
86	XX	406	GLU	N-CA-C	5.31	116.76	111.07
19	5	2695	A	P-O3'-C3'	5.26	128.09	120.20
19	5	4170	A	P-O3'-C3'	5.25	128.08	120.20
19	5	417	G	O4'-C1'-N9	5.24	116.06	108.20
29	A	15	VAL	N-CA-C	-5.22	108.75	113.71
39	K	1664	A	P-O3'-C3'	5.21	128.02	120.20
43	O	110	PRO	N-CA-C	5.20	117.04	110.70
19	5	2661	U	P-O3'-C3'	5.19	127.99	120.20
19	5	4947	U	C2'-C3'-O3'	5.15	121.43	113.70
2	BB	166	VAL	N-CA-C	-5.15	107.96	112.90
39	K	1394	G	C2'-C3'-O3'	5.12	121.38	113.70
86	XX	50	LEU	N-CA-C	5.07	119.16	112.92
39	K	798	G	C4'-C3'-O3'	-5.06	105.41	113.00

There are no chirality outliers.

All (25) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
30	B	257	TRP	Peptide
31	C	339	THR	Peptide
33	E	180	GLY	Peptide
34	F	235	ARG	Peptide
35	G	215	ASP	Peptide
8	HH	32	ILE	Peptide
9	II	99	LEU	Peptide
40	L	4	SER	Peptide
41	M	37	LEU	Peptide
42	N	184	ILE	Peptide
42	N	76	PRO	Peptide
42	N	78	GLY	Peptide
47	S	164	LYS	Peptide
82	TT	54	ASP	Peptide
84	VV	61	GLN	Peptide
85	WW	17	TYR	Peptide

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Mol	Chain	Res	Type	Group
85	WW	37	TYR	Peptide
86	XX	173	TYR	Peptide
86	XX	415	ARG	Mainchain
86	XX	42	PHE	Peptide
87	YY	31	LYS	Peptide
57	b	11	ASN	Peptide
59	d	95	ASP	Peptide
72	q	42	LYS	Peptide
73	r	32	LEU	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	443	0	492	6	0
2	BB	1488	0	1582	21	0
3	CC	1686	0	1772	29	0
4	DD	1525	0	1640	22	0
5	EE	1175	0	1249	10	0
6	FF	488	0	514	4	0
7	GG	795	0	862	13	0
8	HH	636	0	637	8	0
9	II	1190	0	1249	21	0
10	JJ	651	0	672	11	0
11	KK	1068	0	1121	17	0
12	LL	814	0	864	13	0
13	MM	1016	0	1039	14	0
14	0	555	0	567	8	0
15	1	204	0	193	76	0
16	2	1594	0	811	78	0
17	3	1597	0	813	9	0
18	4	127	0	64	0	0
19	5	75972	0	38379	523	0
20	6	2436	0	2393	37	0
21	7	2558	0	1296	16	0
22	8	3208	0	1629	15	0
23	9	459	0	452	9	0
24	NN	1011	0	1083	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	OO	598	0	656	14	0
26	PP	1097	0	1132	22	0
27	QQ	1202	0	1289	8	0
28	RR	908	0	939	5	0
29	A	1898	0	1993	37	0
30	B	3172	0	3310	50	0
31	C	2883	0	3053	31	0
32	D	2391	0	2424	35	0
33	E	1729	0	1887	28	0
34	F	1875	0	1995	28	0
35	G	1879	0	2027	26	0
36	H	1516	0	1597	18	0
37	I	1664	0	1712	20	0
38	J	1362	0	1399	16	0
39	K	36249	0	18308	265	0
40	L	1702	0	1820	25	0
41	M	1137	0	1211	25	0
42	N	1701	0	1749	30	0
43	O	1630	0	1778	26	0
44	P	1242	0	1274	23	0
45	Q	1515	0	1634	26	0
46	R	1508	0	1664	17	0
47	S	1462	0	1508	29	0
48	T	1298	0	1366	21	0
49	U	809	0	833	14	0
50	V	979	0	1039	13	0
51	W	860	0	903	10	0
52	X	967	0	1038	48	0
53	Y	1115	0	1205	19	0
54	Z	1107	0	1182	15	0
55	SS	810	0	836	6	0
56	a	1162	0	1209	26	0
57	b	848	0	920	10	0
58	c	761	0	794	9	0
59	d	888	0	930	6	0
60	e	1053	0	1147	15	0
61	f	876	0	912	15	0
62	g	906	0	998	12	0
63	h	1013	0	1147	21	0
64	i	830	0	916	8	0
65	j	705	0	737	12	0
66	k	569	0	637	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
67	l	447	0	480	27	0
68	m	429	0	465	5	0
69	n	239	0	289	2	0
70	o	851	0	920	12	0
71	p	708	0	756	12	0
72	q	1710	0	1708	22	0
73	r	994	0	1051	12	0
74	s	1507	0	1564	14	0
75	t	1160	0	1218	11	0
76	u	1729	0	1803	26	0
77	v	1716	0	1806	18	0
78	w	1768	0	1866	25	0
79	x	2076	0	2177	25	0
80	y	1471	0	1522	21	0
81	z	1923	0	2089	36	0
82	TT	1034	0	1080	18	0
83	UU	1128	0	1195	19	0
84	VV	1098	0	1167	11	0
85	WW	997	0	1045	17	0
86	XX	3313	0	3425	735	0
87	YY	494	0	527	194	0
88	ZZ	229	0	245	128	0
89	LL	1	0	0	0	0
89	g	1	0	0	0	0
89	j	1	0	0	0	0
89	m	1	0	0	0	0
89	o	1	0	0	0	0
89	p	1	0	0	0	0
90	5	201	0	0	0	0
90	7	7	0	0	0	0
90	8	4	0	0	0	0
90	B	1	0	0	0	0
90	K	78	0	0	0	0
90	P	2	0	0	0	0
90	V	1	0	0	0	0
90	a	1	0	0	0	0
90	e	1	0	0	0	0
90	g	1	0	0	0	0
90	j	1	0	0	0	0
90	y	1	0	0	0	0
All	All	219898	0	164879	2665	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 7.

All (2665) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
86:XX:66:ARG:HH22	86:XX:70:ALA:CA	1.06	1.67
86:XX:19:ILE:HG21	88:ZZ:70:PRO:CD	1.22	1.64
86:XX:19:ILE:CG2	88:ZZ:70:PRO:HD3	1.23	1.59
16:2:48:C:C4	16:2:59:A:C8	1.86	1.57
86:XX:188:CYS:HA	87:YY:44:PHE:CE1	1.35	1.57
86:XX:91:MET:CG	86:XX:116:GLN:HE22	0.97	1.56
86:XX:128:SER:CB	86:XX:155:LEU:HD12	1.36	1.49
86:XX:175:LEU:HB3	86:XX:460:ILE:CG2	1.41	1.48
86:XX:191:ILE:HD12	87:YY:44:PHE:CE1	1.49	1.48
86:XX:19:ILE:HG22	88:ZZ:69:GLY:N	1.22	1.47
86:XX:69:LEU:HD22	86:XX:81:ILE:CG1	1.46	1.44
86:XX:19:ILE:CG2	88:ZZ:69:GLY:H	1.31	1.43
63:h:38:GLY:HA3	86:XX:266:PRO:CG	1.50	1.42
15:1:246:LEU:CD1	19:5:1600:A:H1'	1.51	1.41
87:YY:68:GLY:HA2	88:ZZ:95:ARG:C	1.45	1.41
67:l:21:ARG:HH11	86:XX:273:ARG:CZ	1.32	1.40
86:XX:66:ARG:HD2	86:XX:72:ASN:ND2	1.19	1.40
87:YY:65:ILE:C	88:ZZ:92:LYS:HE2	0.98	1.40
86:XX:259:GLN:HA	86:XX:284:PHE:CE2	1.55	1.40
86:XX:61:PRO:O	86:XX:65:MET:CB	1.69	1.38
19:5:169:A:C2'	19:5:170:C:H5'	1.52	1.37
86:XX:19:ILE:O	88:ZZ:68:VAL:CA	1.70	1.36
86:XX:435:ALA:O	86:XX:441:ILE:CD1	1.74	1.36
63:h:38:GLY:CA	86:XX:266:PRO:HG3	1.55	1.34
86:XX:61:PRO:C	86:XX:65:MET:CE	1.98	1.32
15:1:246:LEU:CD1	19:5:1600:A:O2'	1.78	1.32
16:2:48:C:N4	16:2:59:A:N7	1.77	1.30
86:XX:66:ARG:CD	86:XX:72:ASN:ND2	1.94	1.30
86:XX:259:GLN:HG3	86:XX:284:PHE:CE2	1.64	1.30
86:XX:19:ILE:C	88:ZZ:68:VAL:N	1.87	1.30
86:XX:306:GLN:HE22	86:XX:338:VAL:CG1	1.43	1.28
86:XX:253:ALA:O	87:YY:33:PHE:HE1	1.14	1.28
86:XX:454:ILE:CG2	87:YY:40:THR:HG22	1.64	1.28
86:XX:69:LEU:CB	86:XX:80:GLY:HA2	1.64	1.28
86:XX:69:LEU:HB3	86:XX:80:GLY:CA	1.65	1.27
67:l:21:ARG:HH11	86:XX:273:ARG:NH1	1.32	1.26
86:XX:121:MET:O	86:XX:156:PHE:HE1	1.08	1.26
19:5:2793:G:N3	19:5:2799:G:C2	1.78	1.26

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
86:XX:454:ILE:CG2	87:YY:40:THR:CG2	2.14	1.25
86:XX:69:LEU:CD2	86:XX:81:ILE:CG1	2.15	1.25
86:XX:19:ILE:CG2	88:ZZ:70:PRO:CD	1.92	1.24
86:XX:107:LYS:C	86:XX:108:ASP:N	1.94	1.24
86:XX:91:MET:HG2	86:XX:116:GLN:NE2	0.93	1.24
86:XX:435:ALA:O	86:XX:441:ILE:HD13	1.23	1.24
16:2:48:C:N3	16:2:59:A:C8	2.03	1.23
88:ZZ:74:LEU:O	88:ZZ:78:LEU:CD1	1.85	1.23
86:XX:62:PHE:HA	86:XX:65:MET:SD	1.79	1.23
86:XX:259:GLN:CG	86:XX:284:PHE:CE2	2.21	1.22
86:XX:454:ILE:HG22	87:YY:40:THR:CG2	1.70	1.22
86:XX:153:ILE:O	86:XX:157:VAL:HG23	1.35	1.22
87:YY:68:GLY:HA2	88:ZZ:95:ARG:O	1.36	1.22
86:XX:66:ARG:NH2	86:XX:70:ALA:HA	0.91	1.22
19:5:169:A:O2'	19:5:170:C:H5'	1.35	1.21
86:XX:121:MET:O	86:XX:156:PHE:CE1	1.93	1.21
86:XX:175:LEU:HD23	86:XX:460:ILE:CG2	1.70	1.21
86:XX:292:ILE:HG21	86:XX:449:LEU:CD1	1.71	1.21
86:XX:78:GLU:OE2	86:XX:155:LEU:CD2	1.89	1.21
86:XX:175:LEU:CB	86:XX:460:ILE:HG21	1.69	1.20
67:1:21:ARG:NE	86:XX:273:ARG:HH22	1.37	1.20
86:XX:128:SER:CB	86:XX:155:LEU:CD1	2.19	1.20
88:ZZ:68:VAL:CG1	88:ZZ:70:PRO:O	1.89	1.19
86:XX:46:CYS:SG	86:XX:77:MET:HG3	1.81	1.19
15:1:246:LEU:CD1	19:5:1600:A:C1'	2.19	1.19
86:XX:66:ARG:NH2	86:XX:70:ALA:CA	1.76	1.19
87:YY:65:ILE:O	88:ZZ:92:LYS:CD	1.90	1.19
86:XX:77:MET:C	86:XX:78:GLU:HB2	1.68	1.18
67:1:21:ARG:NH1	86:XX:273:ARG:CZ	2.05	1.18
86:XX:48:ILE:CD1	87:YY:62:ASN:OD1	1.90	1.18
86:XX:69:LEU:CD2	86:XX:81:ILE:HG12	1.73	1.18
86:XX:253:ALA:HB1	87:YY:33:PHE:HZ	1.03	1.17
86:XX:287:SER:HB2	86:XX:452:THR:CG2	1.75	1.17
86:XX:292:ILE:HD13	86:XX:449:LEU:CD1	1.75	1.17
87:YY:65:ILE:CD1	88:ZZ:88:HIS:ND1	2.09	1.16
86:XX:48:ILE:HD12	87:YY:62:ASN:OD1	1.46	1.16
86:XX:61:PRO:C	86:XX:65:MET:SD	2.30	1.15
86:XX:292:ILE:CD1	86:XX:449:LEU:HD22	1.76	1.15
15:1:246:LEU:HD11	19:5:1600:A:C1'	1.74	1.14
86:XX:437:PHE:HD2	86:XX:438:LEU:CD2	1.58	1.14
15:1:246:LEU:HD11	19:5:1600:A:H1'	1.24	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
86:XX:83:PRO:HD3	86:XX:127:GLN:OE1	1.47	1.14
86:XX:443:SER:HB3	86:XX:447:ILE:CD1	1.78	1.14
19:5:169:A:O2'	19:5:170:C:C5'	1.95	1.13
86:XX:191:ILE:HB	87:YY:44:PHE:HZ	1.11	1.13
15:1:246:LEU:HD13	19:5:1600:A:H1'	1.23	1.12
86:XX:69:LEU:HD22	86:XX:81:ILE:HG13	1.28	1.12
67:l:21:ARG:NH1	86:XX:273:ARG:NH1	1.96	1.12
86:XX:132:VAL:HG11	86:XX:151:ILE:HG21	1.13	1.12
86:XX:188:CYS:CA	87:YY:44:PHE:CE1	2.32	1.12
86:XX:259:GLN:CA	86:XX:284:PHE:CE2	2.30	1.12
87:YY:65:ILE:HD12	88:ZZ:88:HIS:ND1	1.62	1.12
52:X:156:ILE:HG12	86:XX:416:TYR:OH	1.50	1.11
86:XX:69:LEU:HD13	86:XX:81:ILE:CD1	1.80	1.11
86:XX:256:ILE:HB	87:YY:36:ILE:HD11	1.29	1.11
86:XX:259:GLN:HG3	86:XX:284:PHE:CZ	1.85	1.11
15:1:246:LEU:HD12	19:5:1600:A:O2'	1.38	1.11
86:XX:175:LEU:CB	86:XX:460:ILE:CG2	2.24	1.10
86:XX:66:ARG:NH1	86:XX:69:LEU:O	1.84	1.09
86:XX:121:MET:HE2	86:XX:160:LEU:HG	1.23	1.09
88:ZZ:68:VAL:HG12	88:ZZ:70:PRO:O	1.43	1.09
15:1:246:LEU:CD1	19:5:1600:A:C2'	2.29	1.09
86:XX:128:SER:HB2	86:XX:155:LEU:HD12	1.11	1.09
87:YY:68:GLY:CA	88:ZZ:95:ARG:C	2.25	1.09
86:XX:43:LEU:HD23	87:YY:50:ILE:HG23	1.32	1.09
86:XX:292:ILE:HD13	86:XX:449:LEU:HD13	1.33	1.09
86:XX:454:ILE:HG22	87:YY:40:THR:HG21	1.27	1.09
86:XX:292:ILE:HD13	86:XX:449:LEU:CG	1.82	1.09
86:XX:287:SER:HB2	86:XX:452:THR:HG21	1.32	1.08
86:XX:454:ILE:HG21	87:YY:40:THR:HG22	1.24	1.08
87:YY:65:ILE:O	88:ZZ:92:LYS:NZ	1.86	1.08
86:XX:253:ALA:O	87:YY:33:PHE:CE1	2.05	1.08
86:XX:91:MET:HG2	86:XX:116:GLN:CD	1.77	1.08
86:XX:259:GLN:HA	86:XX:284:PHE:CZ	1.89	1.08
86:XX:256:ILE:HG13	87:YY:33:PHE:CD1	1.88	1.08
86:XX:292:ILE:HD13	86:XX:449:LEU:CD2	1.82	1.07
86:XX:437:PHE:HD2	86:XX:438:LEU:HD23	1.18	1.07
86:XX:292:ILE:CG1	86:XX:449:LEU:HD13	1.84	1.07
87:YY:66:VAL:HA	88:ZZ:92:LYS:HZ3	1.16	1.07
86:XX:121:MET:CE	86:XX:160:LEU:HG	1.86	1.06
86:XX:192:VAL:HG13	87:YY:52:PHE:CE2	1.90	1.06
86:XX:292:ILE:CD1	86:XX:449:LEU:HD13	1.86	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
86:XX:259:GLN:CB	86:XX:284:PHE:CZ	2.40	1.05
52:X:87:MET:HE2	86:XX:415:ARG:HH22	0.93	1.05
86:XX:69:LEU:CD2	86:XX:81:ILE:HG13	1.82	1.05
86:XX:128:SER:HB3	86:XX:155:LEU:CD1	1.82	1.05
86:XX:61:PRO:C	86:XX:65:MET:HB3	1.81	1.05
87:YY:68:GLY:CA	88:ZZ:95:ARG:O	2.04	1.05
86:XX:69:LEU:HD13	86:XX:81:ILE:CG1	1.87	1.05
86:XX:306:GLN:NE2	86:XX:338:VAL:HG13	1.71	1.05
52:X:87:MET:HE2	86:XX:415:ARG:NH2	1.72	1.04
86:XX:64:TRP:CZ2	86:XX:346:SER:HB2	1.91	1.04
86:XX:306:GLN:NE2	86:XX:338:VAL:CG1	2.21	1.04
86:XX:47:GLN:H	86:XX:75:THR:HB	1.19	1.04
86:XX:66:ARG:HD2	86:XX:72:ASN:CG	1.82	1.04
86:XX:191:ILE:HD12	87:YY:44:PHE:CZ	1.91	1.03
87:YY:66:VAL:C	88:ZZ:92:LYS:HZ1	1.65	1.03
19:5:3901:A:C5	19:5:4450:U:C6	2.46	1.03
86:XX:62:PHE:CA	86:XX:65:MET:SD	2.46	1.03
15:1:258:PRO:O	19:5:4452:U:C2	2.10	1.03
52:X:87:MET:CE	86:XX:415:ARG:HH22	1.69	1.03
86:XX:175:LEU:HD23	86:XX:460:ILE:HG22	1.39	1.03
86:XX:292:ILE:CD1	86:XX:449:LEU:CD2	2.35	1.03
86:XX:441:ILE:C	86:XX:443:SER:N	2.17	1.02
86:XX:252:PHE:CZ	86:XX:451:VAL:HG11	1.95	1.02
88:ZZ:74:LEU:O	88:ZZ:78:LEU:HD13	1.51	1.02
52:X:156:ILE:HG22	87:YY:24:ARG:HE	1.17	1.02
86:XX:253:ALA:HB1	87:YY:33:PHE:CZ	1.93	1.02
15:1:259:LEU:HA	19:5:4452:U:H1'	1.41	1.01
86:XX:69:LEU:HD22	86:XX:81:ILE:HG12	1.33	1.01
86:XX:292:ILE:HG21	86:XX:449:LEU:HD13	1.38	1.01
86:XX:13:CYS:HB3	86:XX:118:LEU:HD11	1.37	1.01
86:XX:175:LEU:CD2	86:XX:460:ILE:CG2	2.39	1.01
86:XX:306:GLN:HE22	86:XX:338:VAL:HG13	1.21	1.01
16:2:48:C:C4	16:2:59:A:N7	2.17	1.01
86:XX:117:LYS:HE2	86:XX:167:GLU:CD	1.84	1.01
86:XX:437:PHE:C	86:XX:438:LEU:HD23	1.84	1.01
15:1:249:TRP:CH2	19:5:3904:G:N2	2.28	1.01
86:XX:189:GLU:OE2	87:YY:50:ILE:HG22	1.60	1.01
86:XX:256:ILE:HB	87:YY:36:ILE:CD1	1.90	1.01
86:XX:191:ILE:CD1	87:YY:44:PHE:CE1	2.43	1.01
86:XX:292:ILE:CG2	86:XX:449:LEU:HD13	1.90	1.01
86:XX:443:SER:HB3	86:XX:447:ILE:CG1	1.90	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
86:XX:191:ILE:HB	87:YY:44:PHE:CZ	1.94	1.00
87:YY:65:ILE:O	88:ZZ:92:LYS:HE3	1.24	1.00
86:XX:69:LEU:HB3	86:XX:80:GLY:HA2	1.02	1.00
88:ZZ:69:GLY:N	88:ZZ:70:PRO:CD	2.25	1.00
86:XX:437:PHE:CD2	86:XX:438:LEU:CD2	2.44	1.00
86:XX:189:GLU:OE2	87:YY:50:ILE:CG2	2.09	1.00
86:XX:369:LEU:HD11	86:XX:430:ALA:HB2	1.42	0.99
86:XX:13:CYS:CB	86:XX:118:LEU:HD11	1.91	0.99
86:XX:309:SER:HG	86:XX:337:PRO:N	1.61	0.99
86:XX:443:SER:HB3	86:XX:447:ILE:HG13	1.42	0.99
86:XX:292:ILE:HG21	86:XX:449:LEU:HD12	1.42	0.99
86:XX:175:LEU:HD23	86:XX:460:ILE:HG23	1.39	0.99
86:XX:69:LEU:CG	86:XX:81:ILE:HG13	1.93	0.98
15:1:250:GLY:HA2	19:5:3908:A:N7	1.78	0.98
67:1:21:ARG:NE	86:XX:273:ARG:NH2	2.10	0.98
86:XX:69:LEU:CD1	86:XX:81:ILE:HG13	1.92	0.98
86:XX:42:PHE:HD1	86:XX:45:CYS:HB2	1.25	0.98
86:XX:69:LEU:HD13	86:XX:81:ILE:HG13	1.42	0.98
86:XX:66:ARG:NH1	86:XX:79:LEU:C	2.22	0.98
87:YY:65:ILE:O	88:ZZ:92:LYS:CE	0.68	0.98
15:1:246:LEU:HD11	19:5:1600:A:O2'	1.53	0.97
86:XX:66:ARG:CZ	86:XX:66:ARG:HA	1.94	0.97
16:2:20:C:H1'	16:2:21:A:OP2	1.64	0.97
86:XX:437:PHE:CD2	86:XX:438:LEU:HD21	2.00	0.97
19:5:169:A:H2'	19:5:170:C:H5'	1.42	0.97
86:XX:19:ILE:CG2	88:ZZ:70:PRO:HD2	1.93	0.97
86:XX:175:LEU:CG	86:XX:460:ILE:HG23	1.95	0.97
86:XX:439:GLY:C	86:XX:440:ALA:N	2.23	0.97
86:XX:175:LEU:CD2	86:XX:460:ILE:HG23	1.94	0.96
16:2:48:C:C5	16:2:59:A:H8	1.84	0.96
86:XX:61:PRO:O	86:XX:65:MET:HB3	0.78	0.95
86:XX:73:ARG:CG	86:XX:131:TYR:OH	2.14	0.95
86:XX:259:GLN:CA	86:XX:284:PHE:HE2	1.73	0.95
86:XX:292:ILE:CB	86:XX:449:LEU:HD13	1.94	0.95
86:XX:42:PHE:CD1	86:XX:45:CYS:HB2	2.00	0.95
86:XX:42:PHE:HE1	86:XX:45:CYS:HG	1.12	0.95
86:XX:47:GLN:O	86:XX:75:THR:CB	2.15	0.95
86:XX:69:LEU:CD1	86:XX:81:ILE:CG1	2.44	0.95
86:XX:128:SER:CA	86:XX:155:LEU:HD12	1.96	0.94
86:XX:259:GLN:CG	86:XX:284:PHE:CZ	2.48	0.94
19:5:2845:A:H61	19:5:3843:C:H42	0.95	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
86:XX:164:LEU:HD13	88:ZZ:73:VAL:HG23	1.48	0.94
86:XX:66:ARG:CD	86:XX:72:ASN:CG	2.38	0.94
86:XX:66:ARG:NE	86:XX:72:ASN:HB3	1.83	0.94
16:2:76:A:H5''	16:2:76:A:H8	1.32	0.94
86:XX:66:ARG:HH11	86:XX:79:LEU:C	1.75	0.93
86:XX:66:ARG:NH2	86:XX:70:ALA:C	2.26	0.93
86:XX:78:GLU:OE2	86:XX:155:LEU:HD22	1.64	0.93
86:XX:185:THR:HA	87:YY:47:MET:HB3	1.51	0.93
86:XX:259:GLN:HA	86:XX:284:PHE:HE2	1.23	0.93
86:XX:86:THR:CG2	86:XX:297:LEU:HD12	1.98	0.93
86:XX:292:ILE:CG2	86:XX:449:LEU:CD1	2.46	0.93
86:XX:121:MET:HE2	86:XX:160:LEU:CG	1.98	0.93
19:5:2845:A:H61	19:5:3843:C:N4	1.67	0.93
17:3:6:G:H1	17:3:67:U:H3	1.12	0.92
86:XX:46:CYS:HA	86:XX:75:THR:OG1	1.70	0.92
86:XX:292:ILE:CD1	86:XX:449:LEU:CD1	2.46	0.92
19:5:3901:A:C5	19:5:4450:U:C5	2.58	0.92
86:XX:191:ILE:HD12	87:YY:44:PHE:HE1	1.33	0.92
86:XX:185:THR:HA	87:YY:47:MET:CB	1.99	0.92
16:2:48:C:C5	16:2:59:A:C8	2.57	0.92
86:XX:62:PHE:N	86:XX:65:MET:SD	2.41	0.92
86:XX:198:PRO:CD	87:YY:55:LYS:HZ3	1.83	0.92
39:K:925:G:H1	39:K:1017:U:H3	1.10	0.91
86:XX:10:LYS:NZ	86:XX:112:PHE:HB2	1.85	0.91
86:XX:259:GLN:CA	86:XX:284:PHE:CZ	2.49	0.91
86:XX:198:PRO:HD3	87:YY:55:LYS:NZ	1.86	0.91
86:XX:69:LEU:CD1	86:XX:81:ILE:HD11	2.00	0.91
86:XX:188:CYS:HA	87:YY:44:PHE:HE1	1.20	0.91
16:2:18:G:O2'	16:2:57:G:N2	2.04	0.91
16:2:21:A:C2	16:2:46:G:C2	2.58	0.91
16:2:48:C:N4	16:2:59:A:C8	2.28	0.90
19:5:2793:G:C4	19:5:2799:G:N1	2.38	0.90
52:X:156:ILE:HG21	86:XX:416:TYR:OH	1.71	0.90
86:XX:69:LEU:HD22	86:XX:81:ILE:CA	1.99	0.90
16:2:48:C:C4	16:2:59:A:H8	1.67	0.90
52:X:156:ILE:CD1	86:XX:415:ARG:NH1	2.35	0.90
86:XX:19:ILE:CB	88:ZZ:70:PRO:CD	2.50	0.90
86:XX:66:ARG:HH21	86:XX:70:ALA:HA	1.34	0.90
16:2:76:A:HO2'	19:5:3909:C:HO2'	0.96	0.90
87:YY:68:GLY:HA2	88:ZZ:96:SER:N	1.86	0.90
88:ZZ:74:LEU:O	88:ZZ:78:LEU:HD12	1.70	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
86:XX:302:TYR:OH	86:XX:341:LEU:HG	1.72	0.89
87:YY:68:GLY:OXT	88:ZZ:92:LYS:HA	1.70	0.89
19:5:3756:A:C2	19:5:3769:C:O2	2.24	0.89
86:XX:259:GLN:CB	86:XX:284:PHE:HZ	1.83	0.89
86:XX:441:ILE:HG13	86:XX:443:SER:N	1.87	0.89
86:XX:10:LYS:HE3	86:XX:112:PHE:HA	1.53	0.89
67:l:21:ARG:CZ	86:XX:273:ARG:NH2	2.35	0.89
86:XX:259:GLN:HB2	86:XX:284:PHE:HZ	1.34	0.89
86:XX:91:MET:HG3	86:XX:116:GLN:HE22	1.35	0.89
88:ZZ:68:VAL:HG13	88:ZZ:70:PRO:O	1.71	0.89
86:XX:46:CYS:SG	86:XX:77:MET:CG	2.60	0.89
86:XX:69:LEU:HD22	86:XX:81:ILE:N	1.87	0.88
19:5:2793:G:N3	19:5:2799:G:N1	2.06	0.88
19:5:2845:A:N6	19:5:3843:C:H42	1.71	0.88
86:XX:188:CYS:SG	87:YY:47:MET:HB2	2.13	0.88
86:XX:19:ILE:CB	88:ZZ:70:PRO:HD2	2.03	0.88
86:XX:291:ILE:CG2	86:XX:372:CYS:HA	2.03	0.88
86:XX:121:MET:HG2	86:XX:163:LEU:HD11	1.53	0.88
86:XX:19:ILE:HB	88:ZZ:68:VAL:HA	1.54	0.88
86:XX:48:ILE:HD13	87:YY:62:ASN:OD1	1.73	0.88
86:XX:132:VAL:HG11	86:XX:151:ILE:CG2	2.03	0.88
86:XX:291:ILE:HG23	86:XX:372:CYS:HA	1.53	0.88
86:XX:47:GLN:C	86:XX:75:THR:HG22	1.99	0.87
16:2:3:U:H3	16:2:70:G:H1	1.22	0.87
86:XX:61:PRO:C	86:XX:65:MET:HE3	1.46	0.87
86:XX:6:LEU:CD1	86:XX:101:GLU:HG3	2.04	0.87
86:XX:198:PRO:CD	87:YY:55:LYS:NZ	2.37	0.87
86:XX:369:LEU:HB3	86:XX:426:LEU:HD11	1.57	0.87
86:XX:256:ILE:CB	87:YY:36:ILE:HD11	2.04	0.87
87:YY:66:VAL:HA	88:ZZ:92:LYS:NZ	1.87	0.87
19:5:3901:A:N7	19:5:4450:U:C5	2.43	0.87
67:l:21:ARG:CZ	86:XX:273:ARG:HH22	1.87	0.87
86:XX:185:THR:CA	87:YY:47:MET:HB3	2.04	0.86
86:XX:47:GLN:O	86:XX:75:THR:HB	1.74	0.86
86:XX:73:ARG:HG3	86:XX:131:TYR:OH	1.75	0.86
86:XX:91:MET:CG	86:XX:116:GLN:NE2	1.79	0.86
86:XX:69:LEU:HB2	86:XX:81:ILE:H	1.39	0.86
86:XX:188:CYS:HA	87:YY:44:PHE:CD1	2.10	0.86
86:XX:66:ARG:CZ	86:XX:69:LEU:O	2.24	0.86
86:XX:19:ILE:O	88:ZZ:68:VAL:N	0.71	0.86
86:XX:19:ILE:HB	88:ZZ:70:PRO:HD2	1.54	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
86:XX:253:ALA:CB	87:YY:33:PHE:HZ	1.85	0.86
86:XX:47:GLN:N	86:XX:75:THR:HB	1.91	0.86
86:XX:69:LEU:HD13	86:XX:81:ILE:HD11	1.53	0.86
86:XX:69:LEU:HD21	86:XX:81:ILE:HG12	1.57	0.86
86:XX:19:ILE:CG2	88:ZZ:69:GLY:N	2.06	0.86
86:XX:256:ILE:CD1	87:YY:37:ALA:HB2	2.06	0.85
86:XX:442:GLY:C	86:XX:443:SER:HB2	2.01	0.85
86:XX:193:TRP:CZ3	87:YY:55:LYS:CE	2.59	0.85
52:X:156:ILE:HD12	86:XX:415:ARG:NH1	1.92	0.85
86:XX:69:LEU:HD22	86:XX:81:ILE:CB	2.06	0.85
87:YY:68:GLY:OXT	88:ZZ:92:LYS:CA	2.25	0.85
87:YY:66:VAL:CA	88:ZZ:92:LYS:NZ	2.40	0.85
86:XX:259:GLN:CB	86:XX:284:PHE:CE2	2.57	0.85
86:XX:443:SER:CB	86:XX:447:ILE:CD1	2.54	0.85
86:XX:19:ILE:HG22	88:ZZ:69:GLY:CA	2.07	0.85
86:XX:42:PHE:HE1	86:XX:45:CYS:SG	2.00	0.85
87:YY:66:VAL:C	88:ZZ:92:LYS:NZ	2.35	0.84
86:XX:69:LEU:HD23	86:XX:80:GLY:C	2.02	0.84
86:XX:103:GLY:O	86:XX:109:ARG:HG2	1.75	0.84
86:XX:153:ILE:O	86:XX:157:VAL:CG2	2.23	0.84
19:5:3901:A:C5	19:5:4450:U:H6	1.91	0.84
19:5:982:U:H3	19:5:1273:G:H1	1.25	0.84
86:XX:292:ILE:HD13	86:XX:449:LEU:HD22	1.46	0.84
39:K:885:U:H3	39:K:901:G:H1	1.22	0.83
86:XX:10:LYS:HZ1	86:XX:112:PHE:HB2	1.38	0.83
86:XX:66:ARG:HH22	86:XX:70:ALA:C	1.86	0.83
67:l:21:ARG:NE	86:XX:273:ARG:HH12	1.75	0.83
86:XX:77:MET:C	86:XX:78:GLU:CB	2.52	0.83
86:XX:47:GLN:H	86:XX:75:THR:CB	1.92	0.83
86:XX:132:VAL:CG1	86:XX:151:ILE:HG21	2.02	0.83
86:XX:6:LEU:HD11	86:XX:101:GLU:HG3	1.61	0.82
39:K:308:G:H3'	39:K:309:G:C5'	2.09	0.82
86:XX:287:SER:HB2	86:XX:452:THR:HG22	1.61	0.82
19:5:3642:A:HO2'	65:j:2:THR:N	1.76	0.82
86:XX:19:ILE:HG21	88:ZZ:70:PRO:CG	2.09	0.82
86:XX:185:THR:CB	87:YY:47:MET:HB3	2.09	0.82
86:XX:191:ILE:CD1	87:YY:44:PHE:CZ	2.62	0.82
15:1:246:LEU:HD11	19:5:1600:A:C2'	2.03	0.82
16:2:48:C:C2	16:2:59:A:H1'	2.15	0.81
86:XX:292:ILE:CG1	86:XX:449:LEU:CD1	2.58	0.81
86:XX:69:LEU:HB2	86:XX:81:ILE:N	1.94	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
86:XX:441:ILE:CB	86:XX:443:SER:N	2.44	0.81
87:YY:68:GLY:OXT	88:ZZ:92:LYS:HE3	1.80	0.81
19:5:3917:A:H5''	19:5:3917:A:H8	1.45	0.81
39:K:1286:G:H21	39:K:1313:A:H62	1.28	0.81
88:ZZ:71:VAL:HG13	88:ZZ:74:LEU:HD12	1.61	0.81
86:XX:175:LEU:HB3	86:XX:460:ILE:HG23	1.60	0.81
39:K:303:C:C2'	39:K:304:C:H5'	2.11	0.81
86:XX:292:ILE:HD11	86:XX:449:LEU:HD22	1.61	0.81
86:XX:441:ILE:HB	86:XX:443:SER:N	1.96	0.81
86:XX:64:TRP:HZ2	86:XX:346:SER:HB2	1.40	0.80
86:XX:435:ALA:O	86:XX:441:ILE:HD11	1.81	0.80
86:XX:121:MET:CG	86:XX:163:LEU:HD11	2.10	0.80
86:XX:259:GLN:CG	86:XX:284:PHE:HE2	1.93	0.80
86:XX:128:SER:HB3	86:XX:155:LEU:HD13	1.64	0.80
86:XX:198:PRO:HD3	87:YY:55:LYS:HZ3	1.40	0.80
86:XX:256:ILE:HG22	87:YY:36:ILE:HD12	1.62	0.80
86:XX:437:PHE:CD2	86:XX:438:LEU:HD23	2.10	0.80
86:XX:47:GLN:N	86:XX:75:THR:CB	2.45	0.80
86:XX:19:ILE:HG13	88:ZZ:70:PRO:CG	2.12	0.80
86:XX:69:LEU:CD2	86:XX:81:ILE:N	2.45	0.80
15:1:251:ARG:HH11	15:1:251:ARG:HG3	1.46	0.80
15:1:259:LEU:H	15:1:259:LEU:HD22	1.46	0.80
19:5:3692:A:H62	19:5:3823:G:H21	1.29	0.80
67:l:21:ARG:NH1	86:XX:273:ARG:NH2	2.30	0.79
86:XX:193:TRP:CE3	87:YY:55:LYS:HE2	2.17	0.79
86:XX:432:SER:OG	86:XX:448:LEU:HD13	1.82	0.79
86:XX:292:ILE:HD11	86:XX:449:LEU:CD2	2.13	0.79
88:ZZ:69:GLY:N	88:ZZ:70:PRO:HD2	1.97	0.79
15:1:248:GLN:O	15:1:253:GLN:HB2	1.83	0.79
52:X:156:ILE:HG22	87:YY:24:ARG:NE	1.95	0.79
67:l:21:ARG:CZ	86:XX:273:ARG:NH1	2.46	0.79
86:XX:443:SER:HB3	86:XX:447:ILE:HD11	1.62	0.78
67:l:21:ARG:HE	86:XX:273:ARG:NH2	1.76	0.78
86:XX:253:ALA:C	87:YY:33:PHE:HE1	1.90	0.78
15:1:250:GLY:CA	19:5:3908:A:N7	2.47	0.78
15:1:246:LEU:HD13	19:5:1600:A:C1'	1.99	0.78
15:1:250:GLY:HA2	19:5:3908:A:C8	2.18	0.78
39:K:303:C:H2'	39:K:304:C:H5'	1.64	0.78
19:5:3908:A:H2'	19:5:3908:A:N3	1.99	0.78
52:X:156:ILE:CG2	87:YY:24:ARG:HE	1.96	0.78
86:XX:103:GLY:O	86:XX:109:ARG:CG	2.32	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
86:XX:180:SER:O	86:XX:453:ILE:HG21	1.83	0.78
39:K:322:C:H6	39:K:322:C:H5''	1.49	0.78
86:XX:42:PHE:CD1	86:XX:45:CYS:CB	2.67	0.78
39:K:1452:A:H61	39:K:1473:G:H21	1.32	0.78
86:XX:19:ILE:HG22	88:ZZ:70:PRO:HD3	1.59	0.78
86:XX:256:ILE:HG13	87:YY:33:PHE:HD1	1.45	0.77
86:XX:302:TYR:OH	86:XX:337:PRO:HD2	1.83	0.77
86:XX:69:LEU:CD1	86:XX:81:ILE:CD1	2.53	0.77
86:XX:369:LEU:HD11	86:XX:430:ALA:CB	2.15	0.77
86:XX:117:LYS:CE	86:XX:167:GLU:CD	2.58	0.77
86:XX:256:ILE:CB	87:YY:36:ILE:CD1	2.61	0.77
87:YY:65:ILE:HD11	88:ZZ:88:HIS:ND1	1.98	0.77
52:X:156:ILE:HD11	86:XX:415:ARG:NH1	2.00	0.77
52:X:151:ASN:HD21	87:YY:20:ARG:CZ	1.96	0.77
86:XX:193:TRP:HZ3	87:YY:55:LYS:HD3	1.48	0.77
86:XX:256:ILE:HD12	87:YY:33:PHE:O	1.85	0.77
86:XX:441:ILE:HD12	86:XX:444:GLY:CA	2.15	0.77
86:XX:69:LEU:CD2	86:XX:80:GLY:C	2.58	0.76
87:YY:65:ILE:HG21	88:ZZ:88:HIS:HE1	1.50	0.76
86:XX:309:SER:OG	86:XX:337:PRO:N	2.19	0.76
52:X:156:ILE:CG1	86:XX:416:TYR:OH	2.31	0.76
86:XX:294:GLN:HB3	86:XX:375:PHE:CD2	2.21	0.76
86:XX:435:ALA:HB1	86:XX:444:GLY:HA2	1.67	0.76
86:XX:66:ARG:HD3	86:XX:72:ASN:ND2	2.00	0.76
67:l:21:ARG:HE	86:XX:273:ARG:HH22	1.27	0.75
67:l:21:ARG:HE	86:XX:273:ARG:NH1	1.83	0.75
15:1:254:PRO:HA	15:1:257:LYS:HE2	1.69	0.75
86:XX:47:GLN:C	86:XX:75:THR:CG2	2.59	0.75
86:XX:69:LEU:CB	86:XX:80:GLY:CA	2.40	0.75
15:1:258:PRO:O	19:5:4452:U:N3	2.20	0.75
67:l:21:ARG:CZ	86:XX:273:ARG:CZ	2.65	0.75
86:XX:10:LYS:HE3	86:XX:112:PHE:CA	2.16	0.75
86:XX:187:ILE:HD12	86:XX:450:ALA:HB2	1.67	0.75
16:2:19:G:H2'	16:2:19:G:N3	2.01	0.75
16:2:20:C:C1'	16:2:21:A:OP2	2.35	0.75
52:X:156:ILE:OXT	86:XX:415:ARG:NH2	2.18	0.75
15:1:246:LEU:HD12	19:5:1600:A:C2'	2.07	0.75
86:XX:443:SER:CB	86:XX:447:ILE:HD11	2.16	0.75
87:YY:68:GLY:OXT	88:ZZ:92:LYS:CE	2.35	0.75
86:XX:365:ILE:HG23	86:XX:433:VAL:HG21	1.68	0.74
86:XX:369:LEU:CD1	86:XX:430:ALA:HB2	2.17	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
86:XX:66:ARG:NH2	86:XX:69:LEU:O	2.20	0.74
88:ZZ:74:LEU:C	88:ZZ:78:LEU:HD13	2.12	0.74
86:XX:73:ARG:CB	86:XX:131:TYR:OH	2.35	0.74
86:XX:259:GLN:HB2	86:XX:284:PHE:CZ	2.14	0.74
16:2:18:G:H2'	16:2:57:G:H22	1.52	0.74
86:XX:64:TRP:CH2	86:XX:346:SER:HA	2.22	0.74
86:XX:306:GLN:HE22	86:XX:338:VAL:HG12	1.46	0.74
86:XX:441:ILE:CG1	86:XX:443:SER:N	2.50	0.74
19:5:1638:A:C6	65:j:8:PHE:HE2	2.06	0.74
19:5:169:A:O2'	19:5:170:C:H5''	1.87	0.74
19:5:1353:G:N7	45:Q:104:ARG:NH2	2.35	0.74
52:X:151:ASN:HD21	87:YY:20:ARG:NH2	1.86	0.74
86:XX:20:GLN:O	88:ZZ:69:GLY:N	2.20	0.74
86:XX:67:VAL:HG13	86:XX:446:GLY:HA3	1.68	0.74
86:XX:103:GLY:O	86:XX:109:ARG:CD	2.35	0.74
88:ZZ:71:VAL:N	88:ZZ:72:PRO:HD2	2.02	0.74
86:XX:121:MET:SD	86:XX:163:LEU:HD11	2.27	0.73
86:XX:256:ILE:CG1	87:YY:33:PHE:CD1	2.70	0.73
67:l:21:ARG:NE	86:XX:273:ARG:NH1	2.36	0.73
86:XX:444:GLY:O	86:XX:446:GLY:N	2.21	0.73
87:YY:68:GLY:HA2	88:ZZ:96:SER:CA	2.19	0.73
15:1:255:ALA:O	19:5:4451:G:N1	2.20	0.73
86:XX:442:GLY:C	86:XX:443:SER:N	2.47	0.73
86:XX:188:CYS:SG	87:YY:44:PHE:HA	2.29	0.73
86:XX:369:LEU:O	86:XX:426:LEU:HD12	1.87	0.73
86:XX:443:SER:N	86:XX:447:ILE:HD12	2.02	0.72
39:K:872:A:C6	39:K:914:U:O4	2.42	0.72
67:l:21:ARG:CZ	86:XX:273:ARG:HH12	2.01	0.72
86:XX:60:ASP:OD2	86:XX:307:MET:SD	2.46	0.72
86:XX:66:ARG:HD2	86:XX:72:ASN:HD22	0.91	0.72
86:XX:86:THR:HG23	86:XX:297:LEU:HD12	1.71	0.72
86:XX:287:SER:CB	86:XX:452:THR:CG2	2.63	0.72
86:XX:117:LYS:HE2	86:XX:167:GLU:OE1	1.88	0.72
86:XX:256:ILE:HD11	87:YY:37:ALA:HB2	1.70	0.72
19:5:2793:G:C4	19:5:2799:G:C2	2.72	0.72
86:XX:69:LEU:HB2	86:XX:80:GLY:HA2	1.68	0.72
86:XX:91:MET:HE3	86:XX:116:GLN:HA	1.71	0.72
86:XX:175:LEU:HB3	86:XX:460:ILE:HG21	0.73	0.72
86:XX:248:THR:OG1	86:XX:440:ALA:C	2.17	0.72
86:XX:256:ILE:HG13	87:YY:33:PHE:CE1	2.24	0.72
87:YY:68:GLY:C	88:ZZ:92:LYS:O	2.31	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:l:21:ARG:HE	86:XX:273:ARG:CZ	2.02	0.72
86:XX:244:ASN:ND2	86:XX:439:GLY:O	2.23	0.72
86:XX:128:SER:HB2	86:XX:155:LEU:CD1	2.02	0.72
15:1:259:LEU:H	15:1:259:LEU:CD2	2.03	0.71
39:K:308:G:H3'	39:K:309:G:H5'	1.70	0.71
86:XX:121:MET:SD	86:XX:163:LEU:CD1	2.78	0.71
86:XX:175:LEU:CG	86:XX:460:ILE:CG2	2.59	0.71
19:5:3901:A:C6	19:5:4450:U:C5	2.79	0.71
86:XX:306:GLN:CD	86:XX:338:VAL:HG13	2.15	0.71
86:XX:78:GLU:OE2	86:XX:155:LEU:HD23	1.89	0.71
87:YY:32:GLU:CD	87:YY:32:GLU:H	1.99	0.71
16:2:48:C:C2	16:2:59:A:C8	2.78	0.71
86:XX:117:LYS:HE2	86:XX:167:GLU:OE2	1.88	0.71
86:XX:193:TRP:CE3	87:YY:55:LYS:CE	2.73	0.71
86:XX:430:ALA:O	86:XX:433:VAL:HB	1.91	0.71
28:RR:33:ARG:HH22	28:RR:89:VAL:HG11	1.55	0.71
86:XX:306:GLN:OE1	86:XX:337:PRO:C	2.34	0.71
16:2:48:C:N3	16:2:59:A:N9	2.38	0.71
87:YY:65:ILE:HG13	88:ZZ:88:HIS:CE1	2.25	0.71
15:1:259:LEU:HA	19:5:4452:U:C1'	2.18	0.70
16:2:48:C:C2	16:2:59:A:C1'	2.74	0.70
86:XX:42:PHE:CE1	86:XX:45:CYS:SG	2.84	0.70
15:1:259:LEU:CA	19:5:4452:U:H1'	2.19	0.70
19:5:3917:A:H5''	19:5:3917:A:C8	2.24	0.70
86:XX:103:GLY:O	86:XX:109:ARG:NE	2.11	0.70
86:XX:309:SER:HB2	86:XX:337:PRO:HD3	1.72	0.70
86:XX:84:ILE:CD1	86:XX:162:VAL:CG1	2.69	0.70
86:XX:175:LEU:CD2	86:XX:460:ILE:HG22	2.12	0.70
86:XX:287:SER:CB	86:XX:452:THR:HG22	2.22	0.70
16:2:76:A:H8	16:2:76:A:C5'	2.02	0.70
87:YY:68:GLY:OXT	88:ZZ:92:LYS:CD	2.40	0.70
76:u:113:MET:HB3	76:u:142:PHE:HE2	1.55	0.70
86:XX:47:GLN:O	86:XX:75:THR:CG2	2.39	0.69
19:5:3896:C:O2'	30:B:268:ARG:NH1	2.26	0.69
61:f:7:CYS:HB2	61:f:103:VAL:HG23	1.74	0.69
86:XX:64:TRP:CD1	86:XX:64:TRP:H	2.06	0.69
9:II:24:ARG:HH22	39:K:1602:U:H4'	1.57	0.69
86:XX:6:LEU:CD1	86:XX:101:GLU:CG	2.70	0.69
86:XX:188:CYS:SG	87:YY:44:PHE:CD1	2.84	0.69
87:YY:68:GLY:HA3	88:ZZ:92:LYS:O	1.92	0.69
88:ZZ:69:GLY:N	88:ZZ:70:PRO:HD3	2.06	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
88:ZZ:79:LEU:C	88:ZZ:79:LEU:HD23	2.18	0.69
19:5:4289:U:HO2'	19:5:4320:G:HO2'	1.38	0.69
31:C:41:HIS:O	31:C:45:ARG:HB2	1.93	0.69
60:e:90:MET:HG2	73:r:33:LYS:HA	1.75	0.69
86:XX:66:ARG:NH2	86:XX:66:ARG:HA	2.07	0.69
86:XX:84:ILE:CD1	86:XX:162:VAL:HG12	2.23	0.69
88:ZZ:78:LEU:HD12	88:ZZ:78:LEU:N	2.07	0.69
86:XX:48:ILE:HG13	86:XX:49:PRO:HD2	1.75	0.69
86:XX:78:GLU:OE2	86:XX:155:LEU:HD21	1.92	0.69
86:XX:47:GLN:N	86:XX:75:THR:HG21	2.07	0.69
86:XX:441:ILE:HD12	86:XX:444:GLY:HA2	1.75	0.68
86:XX:441:ILE:HD12	86:XX:444:GLY:N	2.08	0.68
86:XX:64:TRP:CH2	86:XX:346:SER:CA	2.75	0.68
39:K:872:A:N1	39:K:914:U:O4	2.26	0.68
55:SS:59:LYS:HB3	55:SS:70:TYR:HB2	1.76	0.68
86:XX:124:THR:OG1	86:XX:156:PHE:CE1	2.46	0.68
86:XX:47:GLN:N	86:XX:75:THR:CG2	2.56	0.68
16:2:18:G:C2'	16:2:57:G:N2	2.56	0.68
2:BB:69:LEU:HG	2:BB:96:ALA:HB2	1.75	0.68
86:XX:19:ILE:HG22	88:ZZ:70:PRO:CD	2.17	0.68
88:ZZ:76:MET:SD	88:ZZ:76:MET:N	2.65	0.68
68:m:71:ARG:HE	68:m:96:ARG:HB3	1.59	0.68
86:XX:67:VAL:CG1	86:XX:446:GLY:HA3	2.22	0.68
86:XX:256:ILE:HB	87:YY:36:ILE:CG1	2.24	0.68
67:l:21:ARG:HE	86:XX:273:ARG:HH12	1.37	0.67
86:XX:192:VAL:HG11	87:YY:48:GLY:O	1.94	0.67
87:YY:68:GLY:HA2	88:ZZ:96:SER:HA	1.75	0.67
19:5:2483:G:H1	19:5:2495:U:H3	1.42	0.67
86:XX:47:GLN:O	86:XX:75:THR:HG22	1.93	0.67
88:ZZ:78:LEU:HD12	88:ZZ:78:LEU:H	1.59	0.67
19:5:4884:G:N7	33:E:275:ARG:NH2	2.42	0.67
52:X:156:ILE:CG2	86:XX:416:TYR:OH	2.42	0.67
86:XX:10:LYS:HB3	86:XX:111:LEU:HB3	1.75	0.67
86:XX:406:GLU:OE1	86:XX:407:THR:N	2.27	0.67
19:5:1521:C:OP1	31:C:100:ARG:NH2	2.26	0.67
86:XX:128:SER:HA	86:XX:155:LEU:CD1	2.24	0.67
86:XX:69:LEU:HD11	86:XX:81:ILE:HD11	1.76	0.67
16:2:55:U:O5'	16:2:55:U:H6	1.78	0.67
86:XX:188:CYS:HG	87:YY:44:PHE:HD1	1.40	0.67
13:MM:146:ARG:NH2	39:K:1858:G:OP2	2.28	0.67
19:5:3765:G:O2'	19:5:3766:A:N7	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
77:v:192:LEU:HB3	77:v:227:ARG:HB3	1.76	0.66
86:XX:346:SER:O	86:XX:360:HIS:NE2	2.28	0.66
87:YY:68:GLY:OXT	88:ZZ:92:LYS:CB	2.43	0.66
37:I:87:ILE:HG12	37:I:138:ILE:HG12	1.77	0.66
86:XX:198:PRO:HD2	87:YY:55:LYS:HZ3	1.61	0.66
86:XX:262:ARG:O	87:YY:26:THR:HG22	1.94	0.66
28:RR:54:SER:HB3	28:RR:80:ASP:HA	1.77	0.66
86:XX:191:ILE:CB	87:YY:44:PHE:HZ	2.01	0.66
67:l:21:ARG:NE	86:XX:273:ARG:CZ	2.58	0.66
86:XX:175:LEU:CB	86:XX:460:ILE:HG23	2.11	0.66
87:YY:68:GLY:OXT	88:ZZ:92:LYS:HD2	1.95	0.66
19:5:3769:C:H3'	19:5:3769:C:H6	1.58	0.66
30:B:254:ILE:HG23	30:B:266:VAL:HG11	1.78	0.66
39:K:322:C:H5''	39:K:322:C:C6	2.31	0.66
86:XX:128:SER:CA	86:XX:155:LEU:CD1	2.65	0.66
39:K:1834:A:H2	39:K:1837:G:H1	1.44	0.66
86:XX:45:CYS:HB3	86:XX:77:MET:SD	2.35	0.66
86:XX:73:ARG:HB2	86:XX:131:TYR:OH	1.95	0.66
15:1:250:GLY:C	19:5:3908:A:N7	2.54	0.66
86:XX:259:GLN:HG2	86:XX:284:PHE:CE2	2.28	0.66
86:XX:438:LEU:HD23	86:XX:438:LEU:N	2.03	0.66
16:2:60:A:H8	16:2:60:A:OP2	1.79	0.65
33:E:185:ASN:ND2	33:E:274:LEU:O	2.30	0.65
86:XX:187:ILE:HG21	86:XX:450:ALA:HB3	1.79	0.65
86:XX:432:SER:OG	86:XX:445:THR:HA	1.96	0.65
86:XX:291:ILE:CG2	86:XX:372:CYS:CA	2.73	0.65
13:MM:99:ALA:H	13:MM:133:THR:HG22	1.61	0.65
19:5:1459:A:OP1	45:Q:65:ARG:NH2	2.29	0.65
20:6:298:LEU:HB3	20:6:310:TRP:HB2	1.78	0.65
19:5:2647:A:H62	19:5:2686:G:H8	1.43	0.65
52:X:84:GLU:OE1	86:XX:412:GLU:OE2	2.15	0.65
86:XX:47:GLN:O	86:XX:75:THR:HA	1.96	0.65
86:XX:66:ARG:NH1	86:XX:79:LEU:O	2.23	0.65
86:XX:64:TRP:CZ2	86:XX:346:SER:CB	2.74	0.65
19:5:2406:G:N7	67:l:2:SER:N	2.44	0.65
9:II:121:ARG:NH1	39:K:1611:G:OP2	2.30	0.65
19:5:3901:A:C4	19:5:4450:U:H6	2.15	0.65
86:XX:61:PRO:O	86:XX:65:MET:CG	2.44	0.65
86:XX:66:ARG:HD2	86:XX:72:ASN:CB	2.25	0.65
86:XX:189:GLU:OE2	87:YY:50:ILE:HG21	1.97	0.65
86:XX:442:GLY:C	86:XX:443:SER:CB	2.69	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:2:21:A:C2	16:2:46:G:N2	2.65	0.64
15:1:255:ALA:O	19:5:4451:G:C2	2.51	0.64
88:ZZ:71:VAL:CG1	88:ZZ:74:LEU:HD12	2.27	0.64
15:1:251:ARG:HH11	15:1:251:ARG:CG	2.10	0.64
86:XX:193:TRP:CZ3	87:YY:55:LYS:HE3	2.32	0.64
86:XX:309:SER:CB	86:XX:337:PRO:HD3	2.26	0.64
86:XX:441:ILE:O	86:XX:443:SER:N	2.30	0.64
19:5:3901:A:N6	19:5:4450:U:H5	1.94	0.64
86:XX:67:VAL:HG12	86:XX:68:ILE:HD13	1.80	0.64
86:XX:69:LEU:CB	86:XX:80:GLY:C	2.69	0.64
86:XX:188:CYS:HA	87:YY:44:PHE:CZ	2.19	0.64
3:CC:119:LEU:HD11	3:CC:153:LYS:HG3	1.80	0.64
15:1:259:LEU:O	15:1:260:MET:CB	2.46	0.64
26:PP:60:THR:HG23	26:PP:75:MET:HE2	1.78	0.64
68:m:92:THR:HG22	68:m:94:ASN:H	1.62	0.64
19:5:751:G:H3'	19:5:752:G:H8	1.62	0.64
19:5:1073:G:H1	19:5:1238:A:H2	1.45	0.64
36:H:94:SER:HB3	36:H:142:ASP:HB3	1.80	0.64
86:XX:34:TRP:CZ3	88:ZZ:74:LEU:CD1	2.81	0.64
86:XX:444:GLY:O	86:XX:445:THR:C	2.40	0.64
19:5:941:C:OP2	34:F:241:ARG:NH1	2.31	0.64
39:K:318:A:H61	81:z:186:GLN:HE22	1.43	0.64
80:y:71:ARG:NH1	80:y:148:ASN:OD1	2.31	0.64
86:XX:48:ILE:CG1	86:XX:49:PRO:HD2	2.28	0.64
86:XX:292:ILE:HG12	86:XX:449:LEU:CD1	2.27	0.64
88:ZZ:72:PRO:O	88:ZZ:76:MET:N	2.27	0.64
19:5:4753:U:OP1	61:f:100:ARG:NH1	2.31	0.64
86:XX:252:PHE:CE1	86:XX:451:VAL:HG11	2.33	0.64
20:6:60:ARG:HE	83:UU:97:GLN:HE22	1.46	0.63
22:8:122:G:H21	22:8:128:C:H41	1.44	0.63
39:K:1658:G:OP2	39:K:1660:C:N4	2.31	0.63
53:Y:50:ARG:HB2	53:Y:115:ARG:HH22	1.62	0.63
86:XX:10:LYS:C	86:XX:111:LEU:HD13	2.22	0.63
19:5:2465:C:H1'	19:5:3672:G:H22	1.62	0.63
19:5:3901:A:C6	19:5:4450:U:C6	2.86	0.63
39:K:190:G:O2'	39:K:209:A:N6	2.31	0.63
86:XX:47:GLN:O	86:XX:75:THR:CA	2.46	0.63
86:XX:62:PHE:HB2	86:XX:72:ASN:HD22	1.63	0.63
87:YY:13:GLN:O	87:YY:17:ASP:HB2	1.98	0.63
15:1:257:LYS:H	19:5:4451:G:N2	1.96	0.63
19:5:1824:G:H5''	48:T:35:LYS:HE3	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:M:80:ALA:O	41:M:85:LYS:NZ	2.32	0.63
76:u:82:ARG:NH1	76:u:191:ASP:OD1	2.31	0.63
86:XX:236:ARG:HH12	86:XX:238:ASN:HB2	1.64	0.63
19:5:980:U:H3	19:5:1275:G:H1	1.47	0.63
19:5:1364:U:OP2	40:L:36:ARG:NH2	2.32	0.63
19:5:4398:C:H6	19:5:4398:C:C5'	2.12	0.63
53:Y:8:THR:HG22	53:Y:10:ASP:H	1.63	0.63
86:XX:437:PHE:O	86:XX:438:LEU:HD23	1.98	0.63
32:D:93:THR:O	32:D:158:LYS:NZ	2.32	0.63
39:K:658:U:O2	84:VV:17:ARG:NH2	2.31	0.63
19:5:4280:A:OP2	32:D:23:ARG:NH2	2.31	0.63
30:B:56:ILE:HD11	30:B:368:ILE:HG12	1.81	0.63
86:XX:117:LYS:CE	86:XX:167:GLU:OE1	2.46	0.63
19:5:169:A:C2'	19:5:170:C:C5'	2.49	0.62
39:K:1452:A:H61	39:K:1473:G:N2	1.96	0.62
41:M:104:MET:HE2	43:O:199:HIS:HB3	1.80	0.62
19:5:1654:G:N2	19:5:1678:C:OP1	2.32	0.62
29:A:32:VAL:HG12	29:A:163:ARG:HH22	1.64	0.62
32:D:75:VAL:O	32:D:112:ARG:NH1	2.32	0.62
40:L:116:ARG:NH1	40:L:155:MET:O	2.32	0.62
43:O:18:ARG:HH22	43:O:128:ARG:HH11	1.46	0.62
44:P:118:GLN:HE21	44:P:120:ASN:HD21	1.45	0.62
86:XX:69:LEU:CB	86:XX:81:ILE:N	2.62	0.62
86:XX:253:ALA:CB	87:YY:33:PHE:CZ	2.72	0.62
15:1:249:TRP:CE3	15:1:253:GLN:OE1	2.52	0.62
19:5:2653:C:OP1	62:g:54:ARG:NH2	2.32	0.62
86:XX:6:LEU:HD12	86:XX:101:GLU:HG3	1.79	0.62
86:XX:191:ILE:CB	87:YY:44:PHE:CZ	2.77	0.62
87:YY:66:VAL:O	88:ZZ:92:LYS:NZ	2.25	0.62
19:5:3751:G:H21	19:5:3775:A:H8	1.46	0.62
30:B:59:GLU:HG2	30:B:366:LYS:HD2	1.80	0.62
76:u:144:LYS:HD3	76:u:208:HIS:HB3	1.81	0.62
86:XX:376:SER:HB2	86:XX:421:ALA:HB1	1.82	0.62
15:1:248:GLN:O	15:1:253:GLN:HG3	2.00	0.62
39:K:1286:G:N2	39:K:1313:A:H62	1.95	0.62
86:XX:267:ILE:HG21	86:XX:399:MET:HB3	1.82	0.62
55:SS:3:MET:HG2	55:SS:44:HIS:HD2	1.65	0.62
64:i:48:CYS:SG	64:i:49:GLY:N	2.72	0.62
72:q:10:MET:HE2	72:q:15:VAL:HG22	1.81	0.62
86:XX:42:PHE:CE1	86:XX:45:CYS:CB	2.82	0.62
86:XX:121:MET:HE3	86:XX:156:PHE:CD1	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
86:XX:188:CYS:SG	87:YY:44:PHE:O	2.57	0.62
16:2:48:C:C2	16:2:59:A:N9	2.68	0.62
19:5:3901:A:C6	19:5:4450:U:H5	2.18	0.62
19:5:4523:A:H5''	19:5:4524:G:H5'	1.80	0.62
19:5:4635:A:H2	19:5:4663:G:H21	1.48	0.62
86:XX:66:ARG:CD	86:XX:72:ASN:HB3	2.30	0.62
86:XX:193:TRP:CZ3	87:YY:55:LYS:HE2	2.32	0.62
86:XX:256:ILE:CG2	87:YY:36:ILE:CD1	2.77	0.62
86:XX:303:VAL:HG22	86:XX:345:LEU:HD21	1.80	0.62
86:XX:421:ALA:O	86:XX:425:GLY:N	2.33	0.62
20:6:11:LEU:HB2	20:6:307:VAL:HB	1.80	0.62
88:ZZ:83:SER:O	88:ZZ:87:LEU:HB2	2.00	0.62
7:GG:78:ASP:OD2	23:9:44:ARG:NH1	2.32	0.62
15:1:254:PRO:HG3	19:5:4555:U:H2'	1.81	0.62
86:XX:59:ALA:HB3	86:XX:65:MET:SD	2.40	0.62
86:XX:66:ARG:CD	86:XX:72:ASN:HD22	1.82	0.62
86:XX:121:MET:CG	86:XX:163:LEU:CD1	2.78	0.62
10:JJ:51:GLN:OE1	39:K:1014:G:N2	2.33	0.62
12:LL:5:ARG:NH2	39:K:1862:G:O2'	2.32	0.62
86:XX:34:TRP:HZ3	88:ZZ:74:LEU:HD12	1.64	0.62
86:XX:372:CYS:SG	86:XX:425:GLY:O	2.58	0.62
88:ZZ:71:VAL:N	88:ZZ:72:PRO:CD	2.62	0.62
15:1:241:TYR:HD1	15:1:241:TYR:O	1.83	0.61
19:5:2093:G:H22	19:5:2262:G:H1	1.47	0.61
37:I:150:GLU:OE2	37:I:153:ARG:NH1	2.32	0.61
39:K:153:G:N3	81:z:13:GLN:NE2	2.48	0.61
86:XX:185:THR:HB	87:YY:47:MET:HB3	1.81	0.61
86:XX:302:TYR:CZ	86:XX:341:LEU:HG	2.35	0.61
86:XX:441:ILE:HB	86:XX:444:GLY:H	1.63	0.61
19:5:278:G:H5''	42:N:8:GLN:HE22	1.65	0.61
40:L:48:PRO:HB2	63:h:120:ALA:HB2	1.82	0.61
40:L:56:ARG:O	40:L:116:ARG:NH2	2.33	0.61
86:XX:69:LEU:CG	86:XX:81:ILE:CG1	2.67	0.61
86:XX:121:MET:HG2	86:XX:163:LEU:CD1	2.27	0.61
33:E:48:ARG:HB2	33:E:64:MET:HE1	1.81	0.61
86:XX:47:GLN:HB2	87:YY:58:HIS:CD2	2.35	0.61
86:XX:19:ILE:CG2	88:ZZ:69:GLY:CA	2.74	0.61
86:XX:444:GLY:O	86:XX:447:ILE:N	2.31	0.61
11:KK:5:ARG:NH1	39:K:1455:A:OP1	2.32	0.61
16:2:72:C:H3'	16:2:72:C:C6	2.36	0.61
19:5:1396:G:HO2'	19:5:1468:C:HO2'	1.46	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:5:5047:C:O2'	19:5:5050:C:OP2	2.18	0.61
36:H:102:ASN:HB3	36:H:115:ARG:HB2	1.83	0.61
76:u:120:MET:HG3	76:u:142:PHE:HE1	1.64	0.61
11:KK:58:MET:O	11:KK:62:GLN:NE2	2.33	0.61
15:1:259:LEU:CG	15:1:260:MET:H	2.13	0.61
19:5:3604:A:H5''	46:R:71:ARG:HH12	1.64	0.61
30:B:57:VAL:HG22	30:B:73:VAL:HG12	1.83	0.61
86:XX:59:ALA:CB	86:XX:65:MET:SD	2.89	0.61
86:XX:211:GLY:HA3	86:XX:240:PRO:HG2	1.81	0.61
19:5:2083:C:OP2	45:Q:14:ARG:NH2	2.33	0.61
47:S:82:LEU:HB2	47:S:93:MET:HB2	1.81	0.61
86:XX:34:TRP:HZ3	88:ZZ:74:LEU:CD1	2.13	0.61
86:XX:73:ARG:CD	86:XX:131:TYR:OH	2.48	0.61
87:YY:68:GLY:CA	88:ZZ:92:LYS:O	2.49	0.61
86:XX:6:LEU:HD12	86:XX:101:GLU:OE2	2.00	0.61
86:XX:66:ARG:CD	86:XX:72:ASN:CB	2.79	0.61
87:YY:27:LYS:HZ3	87:YY:27:LYS:HB3	1.63	0.61
3:CC:47:ARG:NH1	39:K:446:G:OP2	2.33	0.61
39:K:910:G:OP2	46:R:173:ARG:NH2	2.34	0.61
39:K:943:U:OP1	76:u:214:LYS:NZ	2.34	0.61
52:X:84:GLU:N	86:XX:403:GLY:O	2.34	0.61
86:XX:256:ILE:CG1	87:YY:33:PHE:CE1	2.84	0.61
87:YY:65:ILE:HA	88:ZZ:92:LYS:HG3	1.82	0.61
19:5:4895:C:O2	41:M:132:ARG:NH2	2.34	0.61
34:F:156:ARG:NH2	34:F:211:LYS:O	2.34	0.61
38:J:16:ARG:HH21	38:J:137:PRO:HG3	1.64	0.61
86:XX:48:ILE:HD13	87:YY:62:ASN:CG	2.25	0.61
86:XX:288:ASN:HB3	86:XX:291:ILE:HB	1.83	0.61
16:2:20:C:H5'	16:2:20:C:O2	2.01	0.60
19:5:942:G:OP1	34:F:244:ARG:NH1	2.28	0.60
39:K:1452:A:N6	39:K:1473:G:H21	1.98	0.60
41:M:126:GLU:HG3	43:O:185:VAL:HG21	1.83	0.60
19:5:2046:G:H5'	43:O:60:LYS:HE2	1.83	0.60
17:3:51:G:H1	17:3:63:C:H42	1.49	0.60
20:6:256:ILE:HB	20:6:270:LEU:HB2	1.83	0.60
23:9:12:ARG:NH1	39:K:1262:C:O2'	2.35	0.60
86:XX:19:ILE:HG13	88:ZZ:70:PRO:HG3	1.81	0.60
86:XX:20:GLN:O	88:ZZ:69:GLY:CA	2.50	0.60
52:X:156:ILE:HG21	86:XX:416:TYR:HH	1.66	0.60
86:XX:19:ILE:C	88:ZZ:68:VAL:CA	2.58	0.60
88:ZZ:71:VAL:O	88:ZZ:71:VAL:HG12	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:K:1091:C:HO2'	82:TT:2:VAL:N	1.99	0.60
66:k:33:LYS:HG2	66:k:46:VAL:HG22	1.82	0.60
87:YY:30:ARG:HD3	87:YY:30:ARG:H	1.66	0.60
19:5:1460:C:H5''	45:Q:144:LYS:HG2	1.84	0.60
24:NN:107:ARG:NH2	39:K:492:C:OP2	2.35	0.60
86:XX:50:LEU:O	86:XX:50:LEU:HD23	2.02	0.60
86:XX:61:PRO:O	86:XX:65:MET:SD	2.51	0.60
86:XX:193:TRP:CZ3	87:YY:55:LYS:HD3	2.33	0.60
87:YY:32:GLU:N	87:YY:32:GLU:OE1	2.34	0.60
26:PP:5:THR:HG23	26:PP:7:LYS:H	1.65	0.60
30:B:240:LEU:HB3	30:B:244:THR:HG21	1.84	0.60
38:J:159:LYS:HG2	38:J:163:MET:HE2	1.82	0.60
52:X:84:GLU:HG3	86:XX:404:HIS:ND1	2.12	0.60
86:XX:244:ASN:O	86:XX:440:ALA:HA	2.02	0.60
86:XX:256:ILE:CG2	87:YY:36:ILE:HD12	2.30	0.60
38:J:18:ARG:HG3	38:J:135:GLY:HA3	1.83	0.59
81:z:76:LEU:HD22	81:z:92:ARG:HG2	1.82	0.59
86:XX:84:ILE:HD12	86:XX:162:VAL:HG11	1.84	0.59
86:XX:193:TRP:HZ3	87:YY:55:LYS:CD	2.13	0.59
16:2:76:A:H5''	16:2:76:A:C8	2.24	0.59
19:5:2891:U:OP2	46:R:74:ARG:NH2	2.35	0.59
19:5:3917:A:H8	19:5:3917:A:C5'	2.15	0.59
19:5:4419:U:OP1	19:5:4421:C:N4	2.30	0.59
8:HH:32:ILE:HD12	8:HH:55:ILE:HB	1.84	0.59
19:5:2262:G:OP2	73:r:98:ARG:NH2	2.33	0.59
29:A:234:LYS:HG2	29:A:238:ILE:HD12	1.84	0.59
30:B:44:THR:HG21	30:B:186:ASN:HD22	1.67	0.59
35:G:116:LEU:HD21	42:N:29:GLN:HG3	1.85	0.59
88:ZZ:78:LEU:CD1	88:ZZ:78:LEU:H	2.14	0.59
16:2:2:C:C6	16:2:2:C:H3'	2.37	0.59
19:5:3700:C:O2'	19:5:3774:A:N3	2.33	0.59
39:K:616:A:OP1	84:VV:68:LYS:NZ	2.36	0.59
76:u:122:GLU:O	76:u:165:ARG:NH2	2.35	0.59
19:5:4754:G:N7	33:E:281:THR:OG1	2.36	0.59
86:XX:160:LEU:HA	86:XX:163:LEU:HD12	1.84	0.59
11:KK:42:PRO:HB3	78:w:203:PRO:HG2	1.85	0.59
19:5:134:G:N2	65:j:80:GLU:OE1	2.35	0.59
15:1:259:LEU:O	15:1:260:MET:HB3	2.03	0.59
19:5:54:G:O2'	42:N:108:ARG:NH2	2.35	0.59
19:5:2299:G:O6	31:C:188:ARG:NH2	2.36	0.59
19:5:3688:U:OP2	29:A:198:ARG:NH2	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:5:4126:C:OP1	35:G:90:LYS:NZ	2.33	0.59
34:F:126:LYS:HB2	48:T:133:ALA:HB3	1.85	0.59
36:H:44:GLU:HB3	36:H:58:ASP:HB2	1.84	0.59
44:P:125:MET:HB2	44:P:141:SER:HB3	1.84	0.59
78:w:172:VAL:HG22	78:w:185:LYS:HG2	1.84	0.59
86:XX:187:ILE:CD1	86:XX:450:ALA:HB2	2.33	0.59
19:5:1499:C:OP1	45:Q:150:ARG:NH2	2.36	0.59
19:5:2520:C:H1'	19:5:2640:G:H21	1.67	0.59
19:5:4124:G:N2	35:G:96:GLN:O	2.35	0.59
19:5:4872:G:OP2	41:M:94:LYS:NZ	2.35	0.59
61:f:41:PHE:HE1	61:f:110:ILE:HD11	1.67	0.59
14:0:107:LYS:HB2	14:0:115:SER:HB3	1.84	0.59
19:5:1428:U:H5'	45:Q:42:THR:HB	1.83	0.59
19:5:2758:G:O2'	19:5:2765:A:N3	2.33	0.59
22:8:21:C:OP1	31:C:195:LYS:NZ	2.34	0.59
72:q:102:ARG:HH12	72:q:105:PRO:HD3	1.68	0.59
86:XX:372:CYS:SG	86:XX:426:LEU:HA	2.42	0.59
87:YY:65:ILE:CG1	88:ZZ:88:HIS:CE1	2.86	0.59
16:2:2:C:C6	16:2:2:C:C3'	2.85	0.58
19:5:35:U:O2'	19:5:1525:A:N1	2.35	0.58
19:5:1405:C:H2'	19:5:1406:G:H8	1.68	0.58
26:PP:56:ARG:NH2	26:PP:99:VAL:O	2.36	0.58
86:XX:69:LEU:HD23	86:XX:80:GLY:O	2.02	0.58
86:XX:103:GLY:C	86:XX:109:ARG:CG	2.76	0.58
16:2:72:C:H6	16:2:72:C:H5''	1.68	0.58
19:5:2489:C:O2'	19:5:2491:C:N4	2.35	0.58
72:q:184:ARG:HD3	72:q:191:ARG:HG2	1.85	0.58
79:x:63:LYS:O	79:x:67:GLN:NE2	2.35	0.58
86:XX:66:ARG:HE	86:XX:72:ASN:HB3	1.66	0.58
86:XX:192:VAL:O	87:YY:52:PHE:CZ	2.56	0.58
86:XX:375:PHE:O	86:XX:379:TRP:HB2	2.03	0.58
16:2:2:C:H3'	16:2:2:C:H6	1.69	0.58
16:2:48:C:O2	16:2:59:A:H1'	2.02	0.58
26:PP:84:ARG:NH1	39:K:1605:G:OP1	2.36	0.58
35:G:139:VAL:HG11	35:G:238:LYS:HG3	1.83	0.58
76:u:136:ARG:HB2	76:u:218:LEU:HD11	1.86	0.58
19:5:3901:A:N7	19:5:4450:U:C6	2.68	0.58
86:XX:19:ILE:HG13	88:ZZ:70:PRO:HG2	1.83	0.58
19:5:1502:G:OP1	45:Q:65:ARG:NH1	2.33	0.58
19:5:2322:G:OP1	60:e:36:ARG:NH1	2.36	0.58
19:5:4691:A:H5'	36:H:71:ARG:HE	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:KK:10:LYS:NZ	39:K:1373:C:O2'	2.36	0.58
19:5:4681:A:O2'	43:O:144:GLU:OE2	2.15	0.58
86:XX:86:THR:HG23	86:XX:297:LEU:CD1	2.33	0.58
87:YY:65:ILE:HD12	88:ZZ:88:HIS:CE1	2.34	0.58
24:NN:91:LEU:HD22	24:NN:96:LEU:HD11	1.85	0.58
35:G:199:LEU:HB2	35:G:204:LYS:HB2	1.86	0.58
87:YY:58:HIS:HA	87:YY:61:ILE:HG12	1.84	0.58
1:AA:79:LEU:HD22	84:VV:68:LYS:HG3	1.86	0.58
4:DD:177:ASN:ND2	39:K:560:A:OP2	2.36	0.58
19:5:1613:A:OP1	29:A:181:LYS:NZ	2.36	0.58
34:F:227:VAL:HA	47:S:39:VAL:HG12	1.85	0.58
86:XX:288:ASN:HD22	86:XX:428:ILE:HG13	1.68	0.58
3:CC:123:ARG:NH1	3:CC:134:GLU:OE1	2.36	0.58
17:3:6:G:N2	17:3:67:U:O2	2.30	0.58
19:5:976:G:H1	19:5:1279:A:H2	1.51	0.58
21:7:59:G:H4'	32:D:267:ASN:HD21	1.67	0.58
19:5:1976:G:N7	19:5:2002:A:O2'	2.34	0.57
19:5:2553:A:H2	19:5:2765:A:H62	1.50	0.57
19:5:2580:U:O2	54:Z:76:ASN:ND2	2.37	0.57
19:5:4981:G:O6	30:B:21:ARG:NH2	2.37	0.57
52:X:80:PRO:HA	52:X:98:PHE:HA	1.86	0.57
52:X:156:ILE:HD12	86:XX:415:ARG:CZ	2.34	0.57
77:v:196:ILE:HB	77:v:223:TYR:HB2	1.86	0.57
82:TT:69:LEU:HD21	82:TT:72:CYS:HB2	1.86	0.57
86:XX:71:SER:HB3	86:XX:75:THR:H	1.68	0.57
86:XX:73:ARG:HD3	86:XX:131:TYR:OH	2.04	0.57
12:LL:21:ILE:HD11	12:LL:32:LYS:HG3	1.86	0.57
15:1:257:LYS:O	19:5:4452:U:C5	2.56	0.57
16:2:64:U:H6	16:2:64:U:O5'	1.87	0.57
24:NN:103:SER:OG	24:NN:106:GLN:OE1	2.20	0.57
32:D:120:GLU:O	32:D:248:ARG:NH2	2.29	0.57
52:X:107:HIS:O	52:X:111:GLN:NE2	2.36	0.57
74:s:32:ALA:O	74:s:85:ASN:ND2	2.36	0.57
78:w:135:GLU:HG3	78:w:153:VAL:HG22	1.85	0.57
83:UU:116:ASP:HB3	83:UU:119:LEU:HD23	1.86	0.57
1:AA:129:ASN:ND2	39:K:637:U:O2	2.33	0.57
16:2:76:A:C5'	16:2:76:A:C8	2.85	0.57
19:5:1072:C:H42	19:5:1239:C:H42	1.50	0.57
27:QQ:121:ARG:NH2	39:K:925:G:OP1	2.37	0.57
42:N:64:ILE:HD11	42:N:102:ALA:HA	1.86	0.57
45:Q:67:ILE:HD12	45:Q:96:PRO:HD2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:l:21:ARG:HH22	67:l:24:PRO:HD3	1.68	0.57
19:5:1548:G:O2'	19:5:2812:A:N3	2.36	0.57
19:5:2664:G:OP1	46:R:110:ARG:NH1	2.36	0.57
29:A:117:GLU:HB2	29:A:162:ASN:HB2	1.85	0.57
30:B:222:VAL:O	30:B:343:ARG:NH1	2.37	0.57
54:Z:12:LEU:HB2	54:Z:81:MET:HB3	1.86	0.57
3:CC:22:HIS:HB3	39:K:433:A:H5''	1.86	0.57
25:OO:43:LYS:HG3	39:K:1600:G:H5'	1.87	0.57
33:E:156:LEU:HD11	33:E:198:ILE:HG13	1.86	0.57
62:g:46:CYS:SG	62:g:47:GLY:N	2.77	0.57
19:5:2808:G:O3'	46:R:60:ARG:NH1	2.37	0.57
19:5:4737:G:H5''	19:5:5069:U:H3'	1.86	0.57
30:B:287:ILE:HG12	30:B:331:VAL:HG12	1.87	0.57
44:P:84:PRO:HB2	44:P:87:SER:HB2	1.87	0.57
56:a:72:THR:HG22	56:a:110:LYS:HB3	1.85	0.57
63:h:38:GLY:HA3	86:XX:266:PRO:CD	2.30	0.57
82:TT:11:LEU:HD12	82:TT:74:VAL:HB	1.85	0.57
84:VV:63:ASN:ND2	84:VV:114:ASP:OD1	2.35	0.57
16:2:59:A:N3	16:2:59:A:H2'	2.19	0.57
19:5:3897:G:N2	19:5:3898:G:O6	2.38	0.57
19:5:3901:A:C5	19:5:4450:U:H5	2.18	0.57
24:NN:110:ARG:HE	24:NN:126:GLY:HA3	1.69	0.57
86:XX:86:THR:CG2	86:XX:297:LEU:CD1	2.80	0.57
19:5:758:G:OP1	36:H:54:ARG:NH2	2.38	0.57
19:5:2088:A:OP2	45:Q:38:ARG:NH2	2.38	0.57
19:5:4099:G:H22	19:5:4109:G:H1	1.50	0.57
19:5:4305:G:H1	48:T:87:LYS:HZ2	1.51	0.57
19:5:4910:A:H4'	30:B:95:THR:HG22	1.87	0.57
19:5:5057:C:O2'	59:d:23:ARG:NH2	2.38	0.57
26:PP:3:GLY:N	39:K:1416:C:O2	2.38	0.57
52:X:151:ASN:ND2	87:YY:20:ARG:CZ	2.67	0.57
82:TT:26:LEU:HD11	82:TT:60:LYS:HB3	1.87	0.57
86:XX:71:SER:O	86:XX:79:LEU:HD23	2.05	0.57
86:XX:193:TRP:CZ3	87:YY:55:LYS:CD	2.88	0.57
19:5:228:C:O2'	53:Y:14:ASN:ND2	2.37	0.57
20:6:177:TRP:HA	20:6:184:LEU:HA	1.86	0.57
52:X:156:ILE:CD1	86:XX:415:ARG:CZ	2.83	0.57
86:XX:64:TRP:CD1	86:XX:64:TRP:N	2.73	0.57
4:DD:170:PRO:O	4:DD:175:ARG:NH1	2.37	0.57
16:2:72:C:C6	16:2:72:C:C3'	2.87	0.57
19:5:2793:G:N3	19:5:2799:G:N2	2.46	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
76:u:35:ALA:O	76:u:42:ARG:NH1	2.37	0.57
79:x:68:ARG:HG3	79:x:76:VAL:HG11	1.87	0.56
86:XX:261:PHE:CE1	87:YY:27:LYS:NZ	2.41	0.56
19:5:1895:G:OP1	34:F:95:ARG:NH2	2.37	0.56
25:OO:106:GLN:HE22	80:y:99:ILE:HD11	1.70	0.56
32:D:261:VAL:HG12	32:D:263:LYS:H	1.69	0.56
39:K:1616:U:OP2	85:WW:43:ARG:NH2	2.37	0.56
86:XX:121:MET:SD	86:XX:163:LEU:HD12	2.45	0.56
86:XX:198:PRO:HD3	87:YY:55:LYS:HZ2	1.70	0.56
86:XX:223:ARG:NH1	86:XX:232:GLU:OE1	2.38	0.56
86:XX:301:LEU:HD23	86:XX:304:ILE:HD12	1.87	0.56
2:BB:154:ILE:HB	2:BB:185:VAL:HG22	1.86	0.56
4:DD:136:ARG:NH1	4:DD:159:PHE:O	2.38	0.56
12:LL:11:ALA:HB3	12:LL:33:ASP:HB2	1.87	0.56
19:5:2533:C:OP1	52:X:139:ARG:NH2	2.39	0.56
19:5:3916:G:H5''	19:5:3916:G:H8	1.71	0.56
19:5:4293:U:O2'	70:o:81:ARG:NH2	2.39	0.56
26:PP:6:VAL:O	26:PP:11:GLN:NE2	2.38	0.56
39:K:453:C:O2'	81:z:92:ARG:O	2.22	0.56
80:y:32:ASP:OD2	80:y:146:ARG:NH2	2.38	0.56
86:XX:291:ILE:HD11	86:XX:376:SER:HA	1.88	0.56
86:XX:297:LEU:HD13	86:XX:300:ASN:HD22	1.70	0.56
86:XX:441:ILE:CB	86:XX:444:GLY:H	2.18	0.56
5:EE:104:LYS:O	84:VV:11:ARG:NH2	2.39	0.56
7:GG:80:PHE:HB3	23:9:52:PHE:HB3	1.87	0.56
16:2:20:C:O4'	16:2:21:A:C5'	2.53	0.56
19:5:942:G:OP1	34:F:145:ASN:ND2	2.39	0.56
19:5:5038:A:OP1	51:W:61:LYS:NZ	2.37	0.56
37:I:38:ARG:HD3	37:I:83:ASP:HB2	1.87	0.56
54:Z:9:LYS:HB2	54:Z:25:ILE:HD12	1.87	0.56
86:XX:66:ARG:HD3	86:XX:72:ASN:CG	2.26	0.56
19:5:2562:G:N2	19:5:2565:A:OP2	2.38	0.56
22:8:65:A:O2'	63:h:10:ARG:NH2	2.38	0.56
40:L:133:ALA:O	40:L:135:LYS:NZ	2.39	0.56
44:P:31:GLU:HG2	44:P:60:PHE:HA	1.86	0.56
58:c:50:ASN:ND2	58:c:75:SER:O	2.39	0.56
86:XX:443:SER:HB3	86:XX:447:ILE:HD12	1.83	0.56
11:KK:5:ARG:HB2	11:KK:10:LYS:HE3	1.88	0.56
15:1:259:LEU:HA	19:5:4452:U:C2	2.39	0.56
21:7:85:G:OP1	34:F:221:LYS:NZ	2.33	0.56
32:D:68:ARG:HG3	32:D:73:MET:HE2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:K:878:G:O6	39:K:908:A:N1	2.38	0.56
39:K:880:G:H2'	39:K:881:G:H8	1.71	0.56
42:N:181:HIS:O	42:N:195:ARG:NH2	2.37	0.56
54:Z:2:GLY:N	58:c:67:ALA:O	2.38	0.56
86:XX:187:ILE:HD12	86:XX:450:ALA:CB	2.34	0.56
9:II:75:ARG:HH21	9:II:95:TYR:HB2	1.70	0.56
19:5:267:G:OP1	63:h:109:ARG:NH2	2.36	0.56
19:5:3938:G:N2	19:5:4171:C:OP2	2.39	0.56
19:5:4769:G:H5'	43:O:176:ARG:HD3	1.88	0.56
26:PP:90:SER:OG	39:K:1654:G:OP1	2.23	0.56
77:v:209:VAL:HG21	77:v:233:LEU:HD11	1.88	0.56
86:XX:392:LYS:O	86:XX:396:GLU:HB2	2.04	0.56
2:BB:53:VAL:HG21	2:BB:172:THR:HA	1.88	0.56
19:5:4896:G:H2'	19:5:4897:G:H8	1.70	0.56
23:9:44:ARG:NH2	39:K:1337:C:OP1	2.39	0.56
26:PP:102:ARG:NH1	39:K:1566:G:OP2	2.39	0.56
39:K:11:A:H5'	77:v:113:GLN:HE21	1.70	0.56
86:XX:253:ALA:C	87:YY:33:PHE:CE1	2.74	0.56
2:BB:114:GLN:NE2	39:K:874:G:N3	2.46	0.56
9:II:115:LYS:HE2	9:II:126:PHE:HB2	1.88	0.56
19:5:935(A):G:OP1	41:M:23:LYS:NZ	2.39	0.56
30:B:317:LEU:HB2	30:B:372:SER:HB2	1.88	0.56
52:X:110:LYS:NZ	52:X:121:VAL:O	2.39	0.56
86:XX:196:PHE:HB2	87:YY:52:PHE:CE1	2.41	0.56
86:XX:198:PRO:CD	87:YY:55:LYS:HZ2	2.17	0.56
19:5:4933:C:OP2	33:E:265:LYS:NZ	2.39	0.56
32:D:107:ARG:NH2	32:D:116:ASP:OD1	2.38	0.56
39:K:903:A:H8	39:K:903:A:OP1	1.88	0.56
58:c:48:LEU:HD21	58:c:60:ILE:HG21	1.87	0.56
80:y:51:HIS:ND1	83:UU:82:TYR:OH	2.38	0.56
85:WW:108:LYS:HG2	85:WW:111:MET:HE2	1.88	0.56
86:XX:10:LYS:NZ	86:XX:112:PHE:CB	2.65	0.56
86:XX:69:LEU:HB3	86:XX:80:GLY:N	2.17	0.56
86:XX:121:MET:HE2	86:XX:160:LEU:CD2	2.35	0.56
9:II:124:ARG:HB2	9:II:131:VAL:HG23	1.88	0.55
19:5:4626:A:OP2	30:B:224:LYS:NZ	2.31	0.55
39:K:309:G:P	39:K:309:G:H8	2.29	0.55
41:M:9:VAL:HG11	41:M:66:HIS:HA	1.88	0.55
47:S:76:LYS:NZ	47:S:100:LEU:O	2.37	0.55
86:XX:59:ALA:HB2	86:XX:79:LEU:HD13	1.87	0.55
87:YY:68:GLY:C	88:ZZ:95:ARG:C	2.56	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BB:143:ARG:HB2	2:BB:155:LYS:HB2	1.89	0.55
16:2:45:G:H8	16:2:45:G:O5'	1.88	0.55
19:5:386:A:O2'	53:Y:87:ARG:NH2	2.38	0.55
19:5:726:G:H4'	34:F:65:ARG:HH22	1.70	0.55
19:5:989:U:H3	19:5:1065:G:H1	1.53	0.55
19:5:2848:G:O2'	19:5:3838:U:O4	2.22	0.55
86:XX:124:THR:OG1	86:XX:156:PHE:HE1	1.89	0.55
86:XX:376:SER:OG	86:XX:422:ALA:HA	2.06	0.55
87:YY:68:GLY:CA	88:ZZ:96:SER:HA	2.32	0.55
9:II:39:ARG:NH2	39:K:1629:C:OP1	2.39	0.55
12:LL:4:LYS:NZ	39:K:1863:A:OP2	2.39	0.55
19:5:150:U:H3	35:G:216:PRO:HD2	1.71	0.55
22:8:155:C:OP2	35:G:142:ARG:NH2	2.40	0.55
31:C:159:GLU:HA	31:C:217:ILE:HB	1.88	0.55
36:H:124:ARG:HH21	36:H:165:THR:HG22	1.71	0.55
39:K:161:U:O2'	81:z:87:ARG:NH1	2.37	0.55
19:5:4944:C:N4	61:f:58:VAL:O	2.38	0.55
86:XX:187:ILE:CD1	86:XX:450:ALA:CB	2.85	0.55
86:XX:368:MET:HE2	86:XX:429:GLY:HA2	1.88	0.55
7:GG:26:SER:HB3	7:GG:32:LEU:HB2	1.89	0.55
19:5:510:U:H5''	56:a:86:THR:HG22	1.87	0.55
19:5:4298:A:OP1	45:Q:160:HIS:NE2	2.38	0.55
46:R:174:GLU:O	46:R:178:GLN:NE2	2.40	0.55
74:s:122:THR:HG22	74:s:159:GLN:HG2	1.87	0.55
87:YY:30:ARG:H	87:YY:30:ARG:CD	2.20	0.55
7:GG:26:SER:HB2	7:GG:110:VAL:HA	1.89	0.55
29:A:137:ILE:HD11	29:A:149:LYS:HB3	1.89	0.55
33:E:96:THR:HG22	33:E:109:VAL:HG22	1.89	0.55
34:F:93:ARG:HE	34:F:108:LEU:HD13	1.72	0.55
86:XX:30:GLU:HG2	86:XX:33:LEU:HD12	1.88	0.55
86:XX:306:GLN:HB2	86:XX:337:PRO:N	2.21	0.55
86:XX:441:ILE:HG13	86:XX:443:SER:CA	2.36	0.55
19:5:4077:A:N1	19:5:4171:C:N4	2.54	0.55
23:9:32:ARG:NH1	39:K:1661:A:OP2	2.35	0.55
25:OO:46:ASN:ND2	39:K:1599:U:OP2	2.40	0.55
86:XX:428:ILE:O	86:XX:431:LEU:HB3	2.05	0.55
19:5:1435:G:O2'	19:5:2105:A:N1	2.37	0.55
21:7:19:C:OP2	38:J:154:LYS:NZ	2.39	0.55
23:9:16:GLN:NE2	39:K:1263:U:O2	2.40	0.55
42:N:68:ARG:NH1	42:N:124:ASP:O	2.39	0.55
48:T:119:ALA:HA	48:T:122:LYS:HB2	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
87:YY:65:ILE:CD1	88:ZZ:88:HIS:CE1	2.86	0.55
19:5:3769:C:H3'	19:5:3769:C:C6	2.39	0.55
21:7:117:G:H5'	32:D:256:LYS:HD2	1.88	0.55
35:G:158:GLU:OE1	35:G:166:ARG:NH2	2.39	0.55
72:q:10:MET:HE1	72:q:51:LEU:HB3	1.88	0.55
84:VV:67:ARG:NH1	84:VV:114:ASP:OD2	2.38	0.55
86:XX:188:CYS:HB3	87:YY:44:PHE:O	2.06	0.55
14:0:138:ARG:HG3	14:0:149:CYS:HA	1.87	0.55
19:5:2380:G:H22	19:5:2424:G:H5'	1.72	0.55
36:H:59:LYS:HE3	36:H:66:GLU:HB3	1.88	0.55
52:X:156:ILE:CG2	87:YY:24:ARG:NE	2.64	0.55
85:WW:60:LEU:HD13	85:WW:89:MET:HG3	1.87	0.55
86:XX:453:ILE:O	86:XX:456:GLN:HG3	2.07	0.55
19:5:109:G:OP2	40:L:74:ARG:NH2	2.40	0.54
19:5:1464:C:H5''	57:b:32:LEU:HD12	1.88	0.54
33:E:144:ARG:NH1	61:f:110:ILE:OXT	2.40	0.54
39:K:168:C:OP1	81:z:131:ARG:NH2	2.40	0.54
39:K:1636:G:H8	80:y:164:ARG:HH22	1.55	0.54
57:b:36:ASP:N	57:b:36:ASP:OD1	2.39	0.54
78:w:148:LYS:NZ	78:w:150:MET:SD	2.72	0.54
13:MM:56:VAL:HG12	13:MM:81:VAL:HG23	1.88	0.54
15:1:248:GLN:O	15:1:253:GLN:CB	2.55	0.54
19:5:4451:G:N2	19:5:4452:U:O4	2.40	0.54
22:8:85:U:O4	53:Y:50:ARG:NH2	2.40	0.54
39:K:628:A:N7	78:w:179:GLN:NE2	2.54	0.54
39:K:885:U:O2	39:K:901:G:N2	2.32	0.54
52:X:83:THR:HG23	86:XX:403:GLY:O	2.06	0.54
83:UU:47:LEU:HG	83:UU:50:LYS:HG3	1.90	0.54
87:YY:65:ILE:CA	88:ZZ:92:LYS:HE2	2.18	0.54
3:CC:12:ARG:HE	3:CC:18:ARG:HG2	1.73	0.54
4:DD:162:ARG:NH1	39:K:583:A:OP1	2.39	0.54
19:5:1555:G:O6	71:p:4:ARG:NH2	2.40	0.54
20:6:236:ILE:HG12	20:6:252:THR:HG22	1.89	0.54
76:u:123:ALA:HB2	76:u:165:ARG:HB2	1.90	0.54
40:L:116:ARG:HH22	40:L:157:ILE:HD11	1.73	0.54
82:TT:42:MET:HE2	82:TT:49:GLU:HA	1.88	0.54
86:XX:175:LEU:HG	86:XX:460:ILE:HG23	1.85	0.54
2:BB:138:GLU:OE2	27:QQ:19:ARG:NH1	2.39	0.54
19:5:4997:G:OP1	59:d:83:ARG:NH1	2.40	0.54
38:J:94:LEU:HB3	38:J:98:ASN:HD22	1.71	0.54
42:N:33:LEU:O	42:N:65:ARG:NH1	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:Q:172:ARG:HH22	56:a:59:ARG:HG2	1.72	0.54
85:WW:44:ARG:NH2	85:WW:53:GLN:OE1	2.41	0.54
86:XX:121:MET:O	86:XX:124:THR:OG1	2.25	0.54
9:II:14:ARG:HE	9:II:17:ASN:HA	1.72	0.54
19:5:1449:C:OP1	45:Q:134:ARG:NH2	2.40	0.54
19:5:4254:G:H1	19:5:4257:A:H62	1.56	0.54
26:PP:96:SER:OG	39:K:1568:C:OP1	2.24	0.54
29:A:5:ILE:HG13	29:A:8:GLN:HG3	1.90	0.54
29:A:82:ILE:HD11	29:A:99:GLY:HA3	1.90	0.54
60:e:101:HIS:O	60:e:128:ARG:NH1	2.40	0.54
6:FF:29:GLN:HE22	6:FF:67:ARG:HA	1.73	0.54
19:5:690:C:H4'	73:r:85:ASN:HD22	1.72	0.54
19:5:2703:G:H5'	49:U:113:ARG:HH12	1.72	0.54
19:5:2793:G:O6	19:5:2799:G:O6	1.92	0.54
19:5:4520:G:OP2	30:B:2:SER:N	2.39	0.54
46:R:105:LEU:HD12	46:R:138:LEU:HD22	1.90	0.54
54:Z:51:ARG:HD2	54:Z:65:ARG:HD2	1.89	0.54
80:y:68:ILE:HD12	80:y:112:LEU:HD22	1.90	0.54
81:z:59:GLN:OE1	81:z:72:ARG:NH1	2.37	0.54
86:XX:10:LYS:CE	86:XX:112:PHE:CA	2.85	0.54
86:XX:103:GLY:C	86:XX:109:ARG:HG2	2.31	0.54
2:BB:142:LYS:HB2	82:TT:54:ASP:HB3	1.90	0.54
10:JJ:32:PHE:HZ	27:QQ:61:ALA:HB2	1.73	0.54
11:KK:17:ILE:HD11	11:KK:54:VAL:HA	1.89	0.54
19:5:2458:C:H5''	42:N:67:ARG:HD2	1.90	0.54
25:OO:80:ARG:NH2	39:K:1599:U:OP1	2.41	0.54
25:OO:85:ARG:NH2	39:K:1596:U:OP2	2.39	0.54
26:PP:22:LEU:HD13	26:PP:28:LEU:HD11	1.89	0.54
39:K:1228:A:H2'	39:K:1229:G:C8	2.43	0.54
49:U:28:PRO:HB2	49:U:34:MET:HG2	1.88	0.54
55:SS:35:LEU:HD12	55:SS:40:VAL:HG21	1.90	0.54
79:x:125:LYS:H	79:x:142:HIS:HD2	1.56	0.54
86:XX:66:ARG:HH22	86:XX:69:LEU:C	2.15	0.54
86:XX:303:VAL:HG22	86:XX:345:LEU:CD2	2.38	0.54
88:ZZ:68:VAL:C	88:ZZ:70:PRO:HD2	2.32	0.54
35:G:111:PRO:HD2	35:G:114:ILE:HD12	1.90	0.54
39:K:903:A:H2'	39:K:904:A:C8	2.43	0.54
67:l:28:TRP:O	67:l:33:ASN:ND2	2.40	0.54
86:XX:437:PHE:C	86:XX:437:PHE:CD2	2.86	0.54
12:LL:32:LYS:NZ	39:K:989:C:O2	2.41	0.54
20:6:118:ARG:NH2	20:6:134:THR:OG1	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:7:49:A:H5''	32:D:224:SER:HB3	1.90	0.54
26:PP:83:GLN:HB2	26:PP:93:SER:HB2	1.89	0.54
66:k:35:LYS:HG2	66:k:44:THR:HG22	1.89	0.54
86:XX:306:GLN:CD	86:XX:338:VAL:CG1	2.78	0.54
86:XX:435:ALA:HB1	86:XX:441:ILE:HG21	1.90	0.54
3:CC:10:LYS:O	3:CC:18:ARG:NH1	2.41	0.53
5:EE:69:ARG:NH1	39:K:114:G:OP1	2.42	0.53
19:5:206:U:O2'	19:5:208:A:N7	2.39	0.53
19:5:328:A:OP2	64:i:30:ARG:NH1	2.38	0.53
19:5:346:G:OP1	53:Y:8:THR:OG1	2.26	0.53
19:5:2081:C:H5''	45:Q:11:ARG:HG3	1.89	0.53
20:6:258:ILE:HD11	20:6:268:ASP:HB2	1.90	0.53
24:NN:55:ILE:HG12	24:NN:75:ILE:HG12	1.89	0.53
29:A:124:GLY:O	29:A:128:ARG:NH1	2.42	0.53
38:J:43:LEU:HD13	38:J:117:ILE:HD11	1.89	0.53
39:K:1847:G:O6	69:n:12:ARG:NH2	2.41	0.53
56:a:82:VAL:HG21	56:a:101:ILE:HG12	1.90	0.53
74:s:106:LYS:HG2	74:s:186:GLY:HA3	1.90	0.53
86:XX:61:PRO:HB2	86:XX:65:MET:CB	2.38	0.53
86:XX:252:PHE:CZ	86:XX:451:VAL:CG1	2.82	0.53
19:5:3799:A:OP1	50:V:66:LYS:NZ	2.36	0.53
19:5:4128:A:O2'	35:G:86:GLU:O	2.25	0.53
19:5:4635:A:H8	19:5:5048:A:H61	1.56	0.53
26:PP:83:GLN:NE2	39:K:1627:C:OP1	2.41	0.53
39:K:126:G:OP2	81:z:195:LYS:NZ	2.39	0.53
83:UU:40:GLU:O	83:UU:45:ARG:NH1	2.40	0.53
86:XX:6:LEU:HD12	86:XX:101:GLU:CG	2.37	0.53
86:XX:11:PRO:HA	86:XX:111:LEU:HD13	1.91	0.53
8:HH:20:SER:HB3	8:HH:59:ILE:HD11	1.90	0.53
19:5:1577:G:C5	29:A:181:LYS:HB2	2.43	0.53
19:5:3769:C:C6	19:5:3769:C:C3'	2.91	0.53
30:B:312:LYS:NZ	30:B:368:ILE:O	2.42	0.53
42:N:146:PRO:HB2	63:h:104:THR:HG23	1.90	0.53
79:x:48:LEU:HD23	79:x:61:VAL:HG13	1.90	0.53
83:UU:13:PHE:HA	83:UU:22:VAL:HA	1.89	0.53
4:DD:70:ARG:HH21	4:DD:94:LEU:HD21	1.73	0.53
19:5:667:A:N7	31:C:2:ALA:N	2.56	0.53
19:5:1440:U:OP1	34:F:33:ARG:NH2	2.41	0.53
19:5:3901:A:C4	19:5:4450:U:C6	2.93	0.53
29:A:29:LEU:O	29:A:123:ARG:NH1	2.41	0.53
36:H:89:ARG:NH2	36:H:147:GLU:OE2	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
81:z:58:LYS:HA	81:z:107:SER:HB2	1.90	0.53
86:XX:175:LEU:HD23	86:XX:460:ILE:O	2.07	0.53
4:DD:172:ARG:NH2	39:K:562:U:O4	2.35	0.53
9:II:22:GLY:HA2	9:II:56:ALA:HB3	1.90	0.53
19:5:1350:C:O2	31:C:119:GLN:NE2	2.42	0.53
19:5:4871:C:H5	47:S:170:LYS:HD2	1.74	0.53
24:NN:7:ILE:HD12	24:NN:43:LYS:HD2	1.91	0.53
32:D:62:CYS:HB3	32:D:105:LEU:HD22	1.89	0.53
72:q:108:PHE:HB2	72:q:136:GLU:HB3	1.90	0.53
11:KK:105:MET:HE1	72:q:51:LEU:H	1.73	0.53
19:5:4882:U:OP1	41:M:117:LYS:NZ	2.42	0.53
26:PP:121:ARG:HH22	39:K:1563:G:H5''	1.73	0.53
30:B:89:ILE:HG22	30:B:162:VAL:HG23	1.90	0.53
39:K:104:A:H62	39:K:356:C:H5	1.57	0.53
39:K:490:C:O2'	39:K:574:A:N1	2.39	0.53
40:L:201:GLU:OE2	40:L:205:GLN:NE2	2.41	0.53
80:y:50:PRO:HG2	80:y:90:VAL:HG22	1.91	0.53
3:CC:113:TYR:OH	3:CC:156:ALA:O	2.25	0.53
7:GG:60:THR:HG22	7:GG:83:ARG:HG2	1.91	0.53
9:II:117:ILE:HG22	85:WW:108:LYS:HD2	1.90	0.53
19:5:2810:U:H5''	46:R:70:ARG:HH22	1.74	0.53
32:D:22:ARG:HE	32:D:27:LYS:HB2	1.74	0.53
39:K:496:C:OP1	79:x:49:ARG:NH1	2.41	0.53
63:h:8:ASP:OD1	63:h:8:ASP:N	2.36	0.53
72:q:37:TYR:OH	72:q:57:LYS:NZ	2.37	0.53
83:UU:51:LEU:HD21	83:UU:81:ILE:HG23	1.90	0.53
86:XX:10:LYS:HZ2	86:XX:112:PHE:HB2	1.68	0.53
86:XX:73:ARG:HD3	86:XX:131:TYR:HH	1.74	0.53
86:XX:117:LYS:NZ	86:XX:167:GLU:CD	2.67	0.53
19:5:3811:G:O2'	19:5:3814:U:OP2	2.26	0.53
35:G:219:LEU:HD21	42:N:45:PRO:HG2	1.90	0.53
41:M:11:ARG:HD2	41:M:57:LEU:HD12	1.91	0.53
71:p:38:THR:HA	71:p:45:THR:HA	1.90	0.53
2:BB:146:VAL:HG22	2:BB:152:ARG:HG2	1.90	0.53
15:1:246:LEU:CD2	15:1:246:LEU:N	2.72	0.53
39:K:476:A:N3	39:K:488:U:O2'	2.35	0.53
39:K:925:G:N2	39:K:1017:U:O2	2.36	0.53
57:b:32:LEU:HD13	57:b:43:MET:HE1	1.90	0.53
83:UU:41:MET:N	83:UU:41:MET:SD	2.82	0.53
87:YY:33:PHE:O	87:YY:37:ALA:HB2	2.08	0.53
9:II:124:ARG:HE	9:II:129:LEU:HB2	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:3:35:A:H2'	17:3:36:A:H8	1.73	0.53
36:H:8:GLN:NE2	36:H:74:CYS:SG	2.82	0.53
71:p:37:TYR:HB2	71:p:47:MET:HB2	1.91	0.53
82:TT:3:ARG:HD3	82:TT:6:VAL:HG22	1.91	0.53
86:XX:66:ARG:NE	86:XX:72:ASN:CB	2.67	0.53
3:CC:190:LEU:HD12	3:CC:194:GLU:HB3	1.90	0.52
7:GG:61:LEU:HB2	7:GG:82:MET:HB3	1.90	0.52
19:5:2411:C:O2'	19:5:2526:C:O2	2.25	0.52
35:G:156:ARG:NH2	35:G:245:ARG:O	2.42	0.52
81:z:54:GLY:O	81:z:110:ASN:ND2	2.42	0.52
87:YY:65:ILE:CG2	88:ZZ:88:HIS:HE1	2.19	0.52
3:CC:178:ARG:HD3	3:CC:181:GLN:HG3	1.89	0.52
14:0:138:ARG:NH1	39:K:1292:C:O2	2.42	0.52
16:2:48:C:H2'	16:2:59:A:O4'	2.09	0.52
19:5:935:A:N1	41:M:70:GLN:NE2	2.57	0.52
19:5:1280:C:O2'	31:C:321:ASN:ND2	2.42	0.52
19:5:1895:G:O2'	19:5:1907:A:N3	2.40	0.52
19:5:4949:G:H4'	19:5:4950:U:H5'	1.91	0.52
86:XX:46:CYS:C	86:XX:75:THR:HG21	2.34	0.52
15:1:258:PRO:O	19:5:4452:U:N1	2.41	0.52
19:5:1985:G:O2'	19:5:2003:G:OP2	2.26	0.52
20:6:133:ASN:HD22	20:6:137:VAL:HB	1.74	0.52
39:K:167:G:O3'	51:W:80:ARG:NH1	2.42	0.52
52:X:147:LEU:CG	87:YY:20:ARG:HH22	2.22	0.52
74:s:102:LEU:HD22	74:s:187:LEU:HD11	1.91	0.52
19:5:46:U:H5''	40:L:16:LYS:HG2	1.92	0.52
24:NN:41:ARG:NH2	24:NN:52:PRO:O	2.42	0.52
30:B:283:LYS:HD3	30:B:363:ILE:HD11	1.91	0.52
31:C:40:VAL:HG22	31:C:115:VAL:HG11	1.91	0.52
78:w:57:ASN:O	78:w:65:ARG:NH1	2.43	0.52
81:z:52:ILE:HD11	81:z:102:VAL:HG21	1.92	0.52
19:5:37:U:H4'	56:a:32:ARG:HD2	1.91	0.52
19:5:2875:C:OP2	71:p:7:LYS:NZ	2.42	0.52
24:NN:104:ARG:NH2	39:K:507:G:OP2	2.43	0.52
39:K:681:U:H4'	84:VV:9:THR:HG22	1.89	0.52
86:XX:248:THR:N	86:XX:440:ALA:CA	2.71	0.52
87:YY:27:LYS:NZ	87:YY:27:LYS:CB	2.73	0.52
87:YY:65:ILE:CG1	88:ZZ:88:HIS:ND1	2.70	0.52
3:CC:33:ALA:HA	39:K:379:C:H5'	1.91	0.52
32:D:119:TYR:HE1	32:D:134:SER:HA	1.75	0.52
39:K:1488:C:O2'	39:K:1490:G:OP2	2.27	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
86:XX:76:LEU:C	86:XX:78:GLU:HG3	2.35	0.52
86:XX:91:MET:HG3	86:XX:116:GLN:NE2	2.03	0.52
86:XX:443:SER:HB2	86:XX:447:ILE:HD11	1.91	0.52
2:BB:101:LEU:O	2:BB:116:ARG:NH1	2.43	0.52
19:5:268:G:H2'	19:5:269:G:H8	1.75	0.52
19:5:667:A:O2'	31:C:29:LYS:NZ	2.43	0.52
19:5:3725:G:N7	64:i:67:LYS:NZ	2.45	0.52
19:5:4874:A:O2'	47:S:170:LYS:NZ	2.43	0.52
86:XX:66:ARG:HH22	86:XX:70:ALA:N	1.94	0.52
86:XX:132:VAL:HG23	86:XX:133:MET:HG3	1.91	0.52
5:EE:99:TYR:O	5:EE:101:ARG:N	2.43	0.52
8:HH:16:LYS:HA	8:HH:23:ILE:HA	1.91	0.52
19:5:3860:A:H61	19:5:4560:C:H5	1.58	0.52
19:5:4519:C:H5''	19:5:4520:G:H5''	1.91	0.52
29:A:120:PRO:HA	29:A:162:ASN:HB3	1.92	0.52
44:P:24:VAL:HG12	44:P:86:LYS:HE2	1.92	0.52
86:XX:19:ILE:HG22	88:ZZ:69:GLY:H	0.43	0.52
88:ZZ:70:PRO:HB2	88:ZZ:72:PRO:HD2	1.92	0.52
4:DD:130:ILE:HG12	4:DD:135:ILE:HD11	1.92	0.52
11:KK:129:LYS:HB2	76:u:150:ILE:HD13	1.90	0.52
19:5:1468:C:OP1	56:a:132:ARG:NH2	2.38	0.52
25:OO:67:LEU:HD13	80:y:103:LEU:HD13	1.92	0.52
39:K:1228:A:H2'	39:K:1229:G:H8	1.75	0.52
61:f:47:CYS:HB3	61:f:103:VAL:HG12	1.92	0.52
62:g:110:GLN:O	62:g:114:GLN:NE2	2.43	0.52
86:XX:125:ILE:N	86:XX:156:PHE:CE1	2.77	0.52
87:YY:68:GLY:OXT	88:ZZ:92:LYS:HB3	2.10	0.52
15:1:259:LEU:HG	15:1:260:MET:H	1.75	0.52
19:5:2305:U:HO2'	60:e:104:SER:HG	1.40	0.52
19:5:2345:G:OP2	56:a:12:ARG:NH1	2.41	0.52
19:5:3901:A:N6	19:5:4450:U:C5	2.77	0.52
42:N:114:ARG:NH1	42:N:151:ILE:O	2.42	0.52
86:XX:19:ILE:CB	88:ZZ:68:VAL:HA	2.32	0.52
86:XX:34:TRP:HH2	88:ZZ:71:VAL:HG21	1.75	0.52
86:XX:128:SER:HA	86:XX:155:LEU:HD12	1.80	0.52
87:YY:30:ARG:CD	87:YY:30:ARG:N	2.73	0.52
4:DD:122:SER:H	4:DD:125:HIS:HB3	1.75	0.51
9:II:28:PHE:HE1	9:II:38:ARG:HE	1.57	0.51
19:5:2280:G:OP1	60:e:48:ARG:NH2	2.43	0.51
30:B:331:VAL:HG21	30:B:347:LEU:HD21	1.92	0.51
78:w:70:THR:HA	78:w:86:LEU:HD13	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
86:XX:86:THR:HG22	86:XX:297:LEU:HB3	1.92	0.51
86:XX:432:SER:HB3	86:XX:445:THR:OG1	2.09	0.51
19:5:158:A:H5''	19:5:159:C:H2'	1.93	0.51
19:5:2486:G:H2'	19:5:2487:G:C8	2.45	0.51
47:S:15:ARG:HH21	48:T:141:VAL:HG22	1.74	0.51
51:W:34:ALA:HA	51:W:37:GLU:HB3	1.92	0.51
79:x:45:ILE:HD12	79:x:80:ILE:HD12	1.92	0.51
86:XX:288:ASN:O	86:XX:291:ILE:N	2.43	0.51
88:ZZ:84:VAL:O	88:ZZ:88:HIS:HB2	2.09	0.51
13:MM:74:ALA:HB1	13:MM:115:ALA:HB2	1.92	0.51
19:5:4398:C:C3'	19:5:4398:C:C6	2.94	0.51
19:5:4939:C:OP1	33:E:190:ARG:NH1	2.43	0.51
21:7:6:C:H4'	32:D:52:ILE:HD13	1.92	0.51
21:7:97:G:O5'	34:F:133:ARG:NH1	2.43	0.51
31:C:140:LYS:HE2	31:C:245:HIS:HB2	1.93	0.51
39:K:116:U:H3	39:K:347:G:H1	1.59	0.51
39:K:429:C:O2'	39:K:811:A:N1	2.41	0.51
54:Z:51:ARG:HB2	54:Z:65:ARG:HD2	1.93	0.51
60:e:26:ASP:OD1	60:e:26:ASP:N	2.40	0.51
78:w:127:MET:HE1	78:w:133:GLY:HA2	1.93	0.51
86:XX:192:VAL:CG1	87:YY:52:PHE:CE2	2.79	0.51
87:YY:27:LYS:HB3	87:YY:27:LYS:NZ	2.25	0.51
88:ZZ:74:LEU:C	88:ZZ:78:LEU:CD1	2.71	0.51
1:AA:107:ARG:HG2	4:DD:32:ILE:HG21	1.92	0.51
19:5:1362:G:OP1	40:L:39:ARG:NH2	2.43	0.51
19:5:4622:A:H4'	30:B:13:SER:HB2	1.91	0.51
19:5:4942:C:OP1	33:E:190:ARG:NH2	2.44	0.51
20:6:292:SER:OG	20:6:293:ALA:N	2.43	0.51
45:Q:78:LYS:HG2	45:Q:137:VAL:HG23	1.92	0.51
76:u:122:GLU:OE2	76:u:213:ARG:NH2	2.40	0.51
86:XX:193:TRP:HE3	87:YY:55:LYS:HE2	1.71	0.51
86:XX:200:THR:HB	86:XX:208:GLU:H	1.74	0.51
9:II:132:ARG:HB2	9:II:134:GLN:HE22	1.76	0.51
11:KK:116:ASN:HD21	72:q:16:LEU:HD13	1.75	0.51
17:3:22:G:H2'	17:3:23:A:H8	1.76	0.51
34:F:104:VAL:HG13	34:F:135:VAL:HG12	1.92	0.51
39:K:96:C:O2	39:K:473:A:O2'	2.27	0.51
39:K:288:G:H1'	79:x:131:VAL:HG21	1.92	0.51
39:K:1208:A:OP2	39:K:1835:A:O2'	2.28	0.51
39:K:1286:G:H21	39:K:1313:A:N6	2.04	0.51
86:XX:248:THR:O	86:XX:251:VAL:HG23	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1:246:LEU:HD23	15:1:246:LEU:H	1.75	0.51
19:5:198:A:OP1	53:Y:126:ARG:NH2	2.43	0.51
19:5:407:A:O2'	19:5:410:A:OP1	2.23	0.51
20:6:29:ASP:OD1	20:6:47:ARG:NH2	2.44	0.51
39:K:860:G:H21	82:TT:107:SER:HB3	1.75	0.51
77:v:110:MET:HB3	77:v:125:LYS:HB3	1.92	0.51
78:w:137:VAL:HG22	78:w:151:LYS:HG3	1.93	0.51
81:z:2:LYS:HB3	81:z:15:LEU:HD21	1.93	0.51
85:WW:44:ARG:NH1	85:WW:48:GLY:O	2.40	0.51
86:XX:62:PHE:N	86:XX:65:MET:CE	2.66	0.51
86:XX:69:LEU:CB	86:XX:81:ILE:HG13	2.39	0.51
86:XX:247:ALA:O	86:XX:251:VAL:HG22	2.10	0.51
3:CC:56:ARG:NH2	39:K:380:G:OP1	2.40	0.51
3:CC:98:LYS:HB3	39:K:377:G:H5'	1.92	0.51
16:2:75:C:N3	19:5:4196:G:C6	2.79	0.51
19:5:2811:G:N1	19:5:2814:C:OP2	2.41	0.51
19:5:4758:U:O2'	43:O:117:ARG:NH1	2.43	0.51
27:QQ:54:LEU:HB3	27:QQ:60:VAL:HG13	1.93	0.51
30:B:41:VAL:HA	30:B:187:GLY:HA3	1.93	0.51
70:o:2:VAL:N	70:o:90:HIS:O	2.43	0.51
86:XX:19:ILE:O	88:ZZ:68:VAL:HA	1.91	0.51
86:XX:306:GLN:NE2	86:XX:338:VAL:HG12	2.13	0.51
33:E:144:ARG:NH2	33:E:194:GLN:O	2.43	0.51
70:o:45:GLN:HE22	70:o:51:GLN:HA	1.75	0.51
86:XX:442:GLY:N	86:XX:443:SER:N	2.58	0.51
2:BB:95:ILE:HD13	2:BB:129:ILE:HG23	1.92	0.51
7:GG:51:LYS:HB2	7:GG:90:ASP:HB2	1.92	0.51
7:GG:94:PRO:HD2	7:GG:97:ILE:HD12	1.92	0.51
19:5:738(A):C:O2'	19:5:740:G:OP2	2.26	0.51
19:5:2631:U:O4	49:U:51:GLY:N	2.42	0.51
19:5:2710:C:H41	46:R:46:LYS:HE3	1.76	0.51
19:5:4305:G:H22	48:T:87:LYS:HZ2	1.59	0.51
39:K:640:A:H2'	39:K:641:A:C8	2.46	0.51
39:K:1757:G:O6	39:K:1775:U:O2	2.29	0.51
54:Z:50:PRO:HD3	54:Z:68:ILE:HG13	1.92	0.51
68:m:68:MET:HG2	68:m:79:PRO:HA	1.93	0.51
86:XX:11:PRO:HA	86:XX:111:LEU:CD1	2.41	0.51
86:XX:13:CYS:HB2	86:XX:118:LEU:HD11	1.86	0.51
86:XX:37:ILE:HA	86:XX:40:PHE:HD2	1.75	0.51
86:XX:369:LEU:C	86:XX:426:LEU:HD12	2.35	0.51
14:0:108:VAL:HG21	28:RR:63:LYS:HG2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:5:3641:U:OP2	19:5:3646:A:N6	2.42	0.51
19:5:4473:A:O2'	68:m:96:ARG:NH2	2.44	0.51
21:7:6:C:O2'	32:D:50:ARG:NH1	2.44	0.51
26:PP:121:ARG:NH1	39:K:1564:C:OP1	2.43	0.51
42:N:108:ARG:HH21	42:N:161:MET:HE2	1.76	0.51
47:S:29:ARG:HB2	48:T:148:PRO:HB2	1.93	0.51
11:KK:19:LYS:HD3	78:w:213:PRO:HD3	1.92	0.50
19:5:71:C:H4'	40:L:67:HIS:HD2	1.74	0.50
19:5:3928:A:OP1	42:N:90:ASN:ND2	2.43	0.50
20:6:127:LYS:HE3	20:6:149:GLU:HA	1.92	0.50
39:K:127:C:O2	79:x:134:LYS:NZ	2.45	0.50
74:s:28:PHE:HB2	74:s:89:VAL:HB	1.94	0.50
83:UU:16:LYS:HE3	83:UU:82:TYR:HD2	1.75	0.50
86:XX:41:ILE:O	86:XX:45:CYS:N	2.30	0.50
86:XX:79:LEU:HD11	86:XX:131:TYR:CE1	2.46	0.50
86:XX:188:CYS:CB	87:YY:47:MET:HB2	2.40	0.50
87:YY:65:ILE:C	88:ZZ:92:LYS:CE	1.90	0.50
9:II:34:LYS:HB3	9:II:103:LEU:HD23	1.92	0.50
11:KK:25:GLY:O	11:KK:31:ASN:ND2	2.44	0.50
19:5:4450:U:O2	19:5:4450:U:O2'	2.17	0.50
39:K:587:A:H5'	39:K:592:C:H41	1.76	0.50
46:R:42:ARG:HA	46:R:45:ILE:HD12	1.93	0.50
86:XX:10:LYS:CE	86:XX:112:PHE:N	2.74	0.50
86:XX:83:PRO:HD3	86:XX:127:GLN:CD	2.30	0.50
86:XX:193:TRP:CE3	87:YY:55:LYS:HE3	2.44	0.50
9:II:35:GLY:O	9:II:97:GLN:NE2	2.44	0.50
19:5:4751:G:H1	19:5:4948:C:H5	1.57	0.50
20:6:238:ALA:H	20:6:251:ALA:HB3	1.76	0.50
28:RR:26:LEU:HG	28:RR:31:LEU:HD21	1.92	0.50
30:B:92:TYR:HB2	30:B:159:VAL:HB	1.94	0.50
31:C:7:LEU:HG	31:C:21:ASN:HB3	1.93	0.50
32:D:279:ARG:HD3	32:D:283:LYS:HE3	1.92	0.50
41:M:97:ALA:HB2	43:O:203:VAL:HB	1.92	0.50
51:W:96:GLN:O	51:W:101:ARG:NH1	2.44	0.50
52:X:84:GLU:CG	86:XX:404:HIS:ND1	2.36	0.50
74:s:77:LYS:O	74:s:81:HIS:ND1	2.43	0.50
81:z:190:ARG:HE	81:z:194:LEU:HD21	1.76	0.50
19:5:709:C:OP1	61:f:89:ARG:NH1	2.44	0.50
19:5:2389:A:H5'	59:d:70:LYS:HE2	1.94	0.50
19:5:4413:C:H5	19:5:4429:C:H42	1.59	0.50
29:A:158:ILE:HG23	29:A:162:ASN:HD21	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:K:1013:U:OP1	39:K:1129:G:O2'	2.30	0.50
39:K:1060:A:O2'	39:K:1062:A:N7	2.38	0.50
41:M:5:ARG:HB3	41:M:57:LEU:HG	1.93	0.50
45:Q:61:LEU:HD21	45:Q:66:MET:HB2	1.93	0.50
70:o:44:LYS:HE2	70:o:52:THR:HB	1.94	0.50
86:XX:72:ASN:HA	86:XX:79:LEU:HA	1.93	0.50
86:XX:373:ALA:O	86:XX:376:SER:OG	2.27	0.50
88:ZZ:81:ILE:C	88:ZZ:81:ILE:HD12	2.36	0.50
4:DD:35:TYR:HD1	4:DD:112:THR:HG21	1.77	0.50
4:DD:133:ARG:NH2	39:K:581:U:OP1	2.44	0.50
19:5:2854:G:O6	30:B:243:LYS:NZ	2.43	0.50
34:F:147:LYS:HB3	34:F:244:ARG:HH11	1.76	0.50
63:h:70:ARG:HB3	63:h:83:LEU:HD22	1.93	0.50
71:p:42:CYS:SG	71:p:59:SER:OG	2.68	0.50
19:5:1492:G:O2'	57:b:41:ARG:NH1	2.45	0.50
19:5:4546:A:N7	29:A:215:ASN:ND2	2.60	0.50
30:B:329:ASP:OD1	30:B:329:ASP:N	2.42	0.50
86:XX:10:LYS:CE	86:XX:112:PHE:HA	2.35	0.50
86:XX:244:ASN:CG	86:XX:439:GLY:O	2.55	0.50
2:BB:117:PRO:HG2	2:BB:120:ARG:HD3	1.93	0.50
15:1:249:TRP:HH2	19:5:3904:G:H21	1.38	0.50
16:2:72:C:H2'	16:2:73:A:H5'	1.93	0.50
19:5:481:G:O2'	19:5:482:G:OP2	2.29	0.50
33:E:204:ILE:HG21	33:E:264:ILE:HG22	1.94	0.50
51:W:56:ARG:HG3	51:W:61:LYS:HB2	1.94	0.50
54:Z:115:LYS:NZ	54:Z:119:GLU:OE2	2.42	0.50
65:j:13:ASN:OD1	65:j:13:ASN:N	2.44	0.50
74:s:58:ASN:HA	74:s:61:MET:HE2	1.94	0.50
79:x:153:LEU:HD13	81:z:216:ARG:HH21	1.77	0.50
86:XX:372:CYS:SG	86:XX:425:GLY:C	2.95	0.50
15:1:258:PRO:O	19:5:4452:U:C4	2.65	0.50
19:5:4454:G:O2'	19:5:4500:U:O2'	2.30	0.50
19:5:4862:G:H2'	19:5:4863:G:C8	2.47	0.50
20:6:107:ASP:HB2	20:6:125:ARG:HD2	1.94	0.50
22:8:12:G:H21	44:P:120:ASN:ND2	2.10	0.50
34:F:231:ASP:OD1	34:F:235:ARG:NH2	2.44	0.50
36:H:91:LYS:HG2	36:H:145:VAL:HG22	1.93	0.50
37:I:17:TYR:H	37:I:95:HIS:HD2	1.59	0.50
39:K:573:U:N3	39:K:576:A:OP2	2.43	0.50
39:K:1033:G:N1	39:K:1080:A:O2'	2.39	0.50
76:u:182:LYS:O	76:u:186:ASN:ND2	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:5:2335:C:H2'	19:5:2336:G:H8	1.76	0.50
39:K:1084:A:OP1	39:K:1858:G:O2'	2.30	0.50
40:L:64:VAL:HA	40:L:67:HIS:CD2	2.47	0.50
80:y:86:LYS:HA	80:y:89:THR:HG22	1.92	0.50
86:XX:61:PRO:HB2	86:XX:65:MET:HB2	1.93	0.50
86:XX:302:TYR:CE2	86:XX:341:LEU:HB3	2.46	0.50
86:XX:461:PHE:O	86:XX:461:PHE:HD1	1.94	0.50
19:5:1881:C:H5'	19:5:2281:U:H1'	1.93	0.49
19:5:4397:A:H2'	19:5:4398:C:H5''	1.94	0.49
19:5:4618:G:H5''	50:V:15:ARG:HB3	1.94	0.49
31:C:218:VAL:HG22	31:C:229:LEU:HG	1.94	0.49
39:K:872:A:N1	39:K:914:U:C4	2.79	0.49
46:R:114:LYS:O	46:R:146:LYS:NZ	2.40	0.49
47:S:34:ALA:HB1	47:S:39:VAL:HG23	1.93	0.49
19:5:107:G:OP2	40:L:42:ARG:NH1	2.44	0.49
19:5:4389:C:H2'	19:5:4390:A:C8	2.48	0.49
33:E:291:PHE:HE2	61:f:110:ILE:HG21	1.76	0.49
42:N:63:ARG:NE	42:N:131:GLU:OE2	2.45	0.49
44:P:3:ARG:NH1	44:P:7:ASP:OD1	2.45	0.49
80:y:14:THR:OG1	80:y:17:ILE:O	2.30	0.49
86:XX:107:LYS:C	86:XX:110:ALA:H	2.20	0.49
86:XX:292:ILE:HG12	86:XX:449:LEU:HD11	1.94	0.49
86:XX:306:GLN:OE1	86:XX:338:VAL:N	2.45	0.49
86:XX:442:GLY:C	86:XX:447:ILE:CD1	2.85	0.49
87:YY:65:ILE:O	88:ZZ:92:LYS:CG	2.57	0.49
88:ZZ:78:LEU:CD1	88:ZZ:78:LEU:N	2.73	0.49
9:II:14:ARG:NH2	38:J:111:GLU:OE2	2.45	0.49
12:LL:44:ILE:HD12	12:LL:45:VAL:HG13	1.94	0.49
16:2:20:C:O2	16:2:20:C:H2'	2.11	0.49
19:5:1907:A:H4'	34:F:222:LYS:HE3	1.94	0.49
32:D:118:ILE:HG12	32:D:138:GLN:HE21	1.77	0.49
33:E:52:LEU:HD13	33:E:53:VAL:HG23	1.93	0.49
39:K:872:A:N6	39:K:914:U:C5	2.81	0.49
74:s:21:LEU:HD13	74:s:75:LEU:HD13	1.94	0.49
86:XX:11:PRO:N	86:XX:111:LEU:HD13	2.27	0.49
86:XX:288:ASN:ND2	86:XX:428:ILE:HG13	2.27	0.49
9:II:127:TRP:O	9:II:144:ARG:NH2	2.45	0.49
11:KK:99:ASP:O	11:KK:102:THR:OG1	2.27	0.49
16:2:48:C:O2'	16:2:59:A:H1'	2.13	0.49
19:5:1326:A:OP2	19:5:4445:U:O2'	2.31	0.49
19:5:4318:C:O2'	70:o:18:HIS:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:5:4348:A:O2'	19:5:4350:C:OP2	2.29	0.49
33:E:153:LEU:HD13	33:E:197:VAL:HG11	1.94	0.49
43:O:77:SER:HB2	43:O:104:VAL:HG12	1.93	0.49
78:w:93:THR:HG21	78:w:198:ILE:HG13	1.95	0.49
86:XX:71:SER:HB2	86:XX:78:GLU:N	2.28	0.49
87:YY:30:ARG:HD3	87:YY:30:ARG:N	2.27	0.49
10:JJ:67:THR:OG1	10:JJ:70:LYS:O	2.30	0.49
19:5:510:U:H5'	56:a:85:GLN:HG3	1.95	0.49
19:5:1563:A:H2'	19:5:1564:A:C8	2.47	0.49
19:5:1757:U:OP1	19:5:1768:C:N4	2.46	0.49
19:5:2503:G:N2	19:5:4084:G:O4'	2.45	0.49
37:I:35:ASP:HB3	37:I:88:ARG:HD2	1.95	0.49
42:N:17:ASP:OD1	42:N:20:ARG:NH2	2.45	0.49
49:U:105:ASN:HB2	49:U:111:GLU:HB2	1.94	0.49
78:w:167:TYR:OH	78:w:202:LYS:O	2.27	0.49
86:XX:184:ALA:HB2	86:XX:453:ILE:CG2	2.42	0.49
86:XX:442:GLY:C	86:XX:443:SER:CA	2.86	0.49
88:ZZ:75:VAL:HA	88:ZZ:78:LEU:HD13	1.94	0.49
19:5:2073:C:H4'	34:F:156:ARG:HH22	1.77	0.49
20:6:70:VAL:HG11	20:6:112:ALA:HA	1.94	0.49
24:NN:104:ARG:HA	24:NN:107:ARG:HE	1.78	0.49
31:C:92:PHE:HB3	31:C:100:ARG:HH12	1.77	0.49
39:K:10:G:H21	77:v:114:LYS:HA	1.78	0.49
49:U:56:LEU:HB3	49:U:61:VAL:HG23	1.95	0.49
54:Z:66:SER:HB2	54:Z:122:TYR:HE2	1.77	0.49
65:j:35:GLY:O	65:j:45:ARG:NH1	2.45	0.49
83:UU:31:LEU:HD12	83:UU:33:LYS:HE3	1.93	0.49
86:XX:84:ILE:CD1	86:XX:162:VAL:HG11	2.41	0.49
86:XX:84:ILE:HD13	86:XX:162:VAL:HG12	1.94	0.49
86:XX:294:GLN:CB	86:XX:375:PHE:CD2	2.94	0.49
19:5:1315:C:OP1	60:e:44:ARG:NH1	2.40	0.49
19:5:2651:C:O2'	62:g:54:ARG:NH2	2.46	0.49
19:5:3717:A:H2'	19:5:3718:A:C8	2.47	0.49
86:XX:367:PHE:O	86:XX:371:SER:OG	2.22	0.49
16:2:20:C:O4'	16:2:21:A:H5'	2.12	0.49
19:5:67:C:OP2	19:5:312:G:N2	2.42	0.49
21:7:48:G:OP1	32:D:226:TYR:OH	2.30	0.49
22:8:141:C:H5'	42:N:113:LEU:HD11	1.93	0.49
39:K:482:G:N1	39:K:485:A:OP2	2.39	0.49
42:N:104:GLU:HA	42:N:160:GLU:HG3	1.94	0.49
86:XX:6:LEU:HD12	86:XX:101:GLU:CD	2.37	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
86:XX:194:LYS:HD2	86:XX:240:PRO:HG3	1.94	0.49
3:CC:144:LYS:NZ	39:K:206:G:O6	2.45	0.49
12:LL:34:LYS:NZ	39:K:1862:G:N7	2.58	0.49
16:2:19:G:N3	16:2:19:G:C2'	2.73	0.49
19:5:280:G:O6	42:N:15:GLN:NE2	2.45	0.49
19:5:2529:A:O2'	19:5:2531:C:OP2	2.29	0.49
19:5:4084:G:O6	29:A:72:ARG:NH2	2.41	0.49
19:5:4737:G:H1	19:5:4962:C:H42	1.60	0.49
20:6:152:SER:OG	20:6:168:CYS:SG	2.64	0.49
39:K:334:C:H5	81:z:190:ARG:HH12	1.60	0.49
39:K:1485:U:OP1	78:w:151:LYS:NZ	2.42	0.49
86:XX:259:GLN:C	86:XX:284:PHE:HE2	2.20	0.49
19:5:4472:G:O2'	68:m:74:TYR:O	2.24	0.49
19:5:4736:C:H2'	19:5:4737:G:H8	1.77	0.49
3:CC:6:ASP:OD1	3:CC:9:HIS:ND1	2.46	0.48
16:2:65:C:H2'	16:2:66:C:C6	2.48	0.48
19:5:722:G:OP1	19:5:935(A):G:N1	2.39	0.48
40:L:43:ALA:O	40:L:149:GLN:NE2	2.45	0.48
43:O:175:MET:HE3	43:O:179:LYS:HE3	1.94	0.48
63:h:37:THR:O	86:XX:266:PRO:CG	2.61	0.48
63:h:38:GLY:HA3	86:XX:266:PRO:HG3	0.62	0.48
65:j:27:TYR:HA	65:j:34:CYS:HA	1.95	0.48
76:u:174:ARG:NH2	76:u:196:ASP:OD2	2.46	0.48
88:ZZ:75:VAL:CA	88:ZZ:78:LEU:HD13	2.43	0.48
19:5:3937:C:H1'	42:N:125:SER:HB3	1.94	0.48
25:OO:110:THR:HG21	80:y:102:LEU:HD22	1.95	0.48
45:Q:70:MET:HE1	45:Q:78:LYS:HB3	1.94	0.48
79:x:11:ARG:NH2	79:x:24:THR:OG1	2.45	0.48
86:XX:164:LEU:HD13	88:ZZ:73:VAL:CG2	2.32	0.48
2:BB:91:HIS:HB2	2:BB:172:THR:HG21	1.93	0.48
4:DD:134:HIS:NE2	39:K:561:A:O2'	2.33	0.48
19:5:2621:A:H62	49:U:81:ARG:HH12	1.60	0.48
26:PP:10:ASN:H	26:PP:142:LYS:HZ1	1.60	0.48
30:B:57:VAL:HB	30:B:367:PHE:HB3	1.94	0.48
34:F:178:LEU:HD21	34:F:203:ALA:HA	1.95	0.48
72:q:63:ARG:HD3	72:q:185:MET:HE1	1.94	0.48
86:XX:193:TRP:HZ2	87:YY:54:VAL:HG23	1.77	0.48
5:EE:57:ASP:OD1	5:EE:84:ARG:NH1	2.46	0.48
19:5:1962:A:H5''	19:5:2024:G:H22	1.78	0.48
19:5:4894:A:H5''	19:5:4895:C:H2'	1.95	0.48
53:Y:72:GLN:HE22	53:Y:74:TYR:HD1	1.60	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
86:XX:47:GLN:CA	86:XX:75:THR:CG2	2.92	0.48
16:2:61:C:C2'	16:2:62:C:H5'	2.43	0.48
19:5:62:A:N3	19:5:77:U:O2'	2.42	0.48
19:5:1990:A:O2'	75:t:99:LYS:NZ	2.46	0.48
19:5:2274:C:H5'	31:C:312:ARG:HB3	1.95	0.48
20:6:118:ARG:HH21	20:6:134:THR:H	1.61	0.48
32:D:150:LEU:HD22	38:J:145:LYS:HE2	1.95	0.48
60:e:7:LEU:HB2	60:e:93:LYS:HB3	1.94	0.48
61:f:81:SER:O	61:f:81:SER:OG	2.27	0.48
86:XX:6:LEU:HB2	86:XX:101:GLU:OE2	2.14	0.48
86:XX:107:LYS:O	86:XX:110:ALA:N	2.45	0.48
86:XX:285:TYR:O	86:XX:286:THR:OG1	2.18	0.48
86:XX:302:TYR:OH	86:XX:337:PRO:CD	2.58	0.48
88:ZZ:79:LEU:C	88:ZZ:79:LEU:CD2	2.85	0.48
19:5:2326:G:OP1	60:e:108:ARG:NH1	2.47	0.48
19:5:4398:C:C6	19:5:4398:C:H3'	2.48	0.48
19:5:4992:G:H2'	19:5:4993:G:C8	2.49	0.48
20:6:167:SER:OG	20:6:177:TRP:NE1	2.40	0.48
24:NN:20:ARG:NH1	79:x:60:GLU:OE1	2.46	0.48
33:E:191:ARG:NH2	33:E:217:ASP:OD1	2.47	0.48
39:K:128:U:H3'	39:K:129:C:H6	1.78	0.48
39:K:918:U:O2'	82:TT:56:HIS:O	2.31	0.48
47:S:154:LEU:HB3	47:S:157:ARG:HD3	1.94	0.48
51:W:6:CYS:HB3	51:W:10:GLY:H	1.78	0.48
66:k:26:LYS:HD3	66:k:69:LEU:HD12	1.95	0.48
4:DD:38:ARG:NH2	39:K:643:A:OP2	2.40	0.48
19:5:2639:U:H2'	19:5:2694:G:H1	1.78	0.48
39:K:466:G:O2'	81:z:72:ARG:NH2	2.44	0.48
85:WW:17:TYR:HE2	85:WW:37:TYR:HB3	1.79	0.48
86:XX:198:PRO:HG3	87:YY:55:LYS:HZ2	1.78	0.48
86:XX:368:MET:HG3	86:XX:429:GLY:HA3	1.95	0.48
87:YY:36:ILE:O	87:YY:40:THR:OG1	2.25	0.48
3:CC:142:SER:OG	3:CC:143:LYS:N	2.47	0.48
6:FF:14:VAL:HG22	6:FF:30:VAL:HG11	1.94	0.48
16:2:18:G:H2'	16:2:57:G:N2	2.19	0.48
16:2:53:G:H2'	16:2:54:U:C6	2.49	0.48
19:5:257:C:H2'	19:5:258:G:H8	1.78	0.48
19:5:3901:A:H62	19:5:4450:U:H5	1.60	0.48
19:5:4387:C:H2'	19:5:4388:A:H8	1.79	0.48
31:C:284:MET:HE2	31:C:287:THR:HA	1.95	0.48
35:G:218:GLU:OE2	42:N:26:ARG:NH1	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:J:24:ILE:HG12	38:J:128:LEU:HB3	1.95	0.48
39:K:303:C:C3'	39:K:304:C:H5'	2.42	0.48
39:K:1693:G:H21	39:K:1834:A:H8	1.62	0.48
80:y:35:LEU:HG	80:y:146:ARG:HH21	1.79	0.48
86:XX:6:LEU:HD11	86:XX:101:GLU:CG	2.39	0.48
86:XX:10:LYS:HE3	86:XX:112:PHE:N	2.29	0.48
3:CC:142:SER:HB3	3:CC:145:ILE:HG22	1.96	0.48
17:3:26:A:H61	17:3:44:G:H1	1.62	0.48
19:5:1638:A:C6	65:j:8:PHE:CE2	2.96	0.48
19:5:2627:C:OP1	49:U:92:LYS:NZ	2.47	0.48
19:5:4138:C:N4	19:5:4146:G:O6	2.40	0.48
39:K:1536:G:H2'	39:K:1537:A:C8	2.48	0.48
39:K:1679:A:H2'	80:y:60:ARG:HD2	1.96	0.48
54:Z:5:MET:O	54:Z:28:ASN:ND2	2.39	0.48
64:i:33:LEU:HD11	64:i:38:LYS:HD2	1.96	0.48
72:q:2:SER:OG	72:q:56:GLU:OE1	2.31	0.48
86:XX:437:PHE:CE2	86:XX:438:LEU:HD21	2.44	0.48
8:HH:14:PRO:HD2	77:v:255:LEU:HD11	1.96	0.48
15:1:243:PRO:HA	15:1:244:PRO:HD3	1.74	0.48
19:5:371:A:N3	19:5:1531:U:O2'	2.42	0.48
19:5:4076:G:OP1	35:G:126:ARG:NE	2.32	0.48
24:NN:7:ILE:HG12	24:NN:27:VAL:HG22	1.96	0.48
39:K:64:A:H2	39:K:83:A:H62	1.60	0.48
39:K:1492:U:O2'	39:K:1495:G:OP1	2.31	0.48
41:M:7:VAL:HG13	41:M:27:ILE:HD13	1.96	0.48
10:JJ:30:SER:OG	39:K:1016:U:O2	2.32	0.47
19:5:368:C:H1'	31:C:82:GLY:HA2	1.96	0.47
19:5:1578:U:H5''	71:p:17:ARG:HH22	1.78	0.47
19:5:2035:C:H5'	47:S:118:ARG:HE	1.79	0.47
19:5:4277:G:O2'	19:5:4282:A:N1	2.42	0.47
19:5:4985:U:O2	30:B:174:ARG:NH1	2.47	0.47
29:A:130:SER:OG	29:A:174:ARG:NH2	2.40	0.47
30:B:291:TYR:OH	30:B:315:ASN:ND2	2.47	0.47
31:C:32:ILE:HD12	31:C:130:ALA:HB2	1.95	0.47
34:F:34:LYS:O	34:F:38:GLN:NE2	2.47	0.47
39:K:1121:G:O2'	76:u:204:ILE:O	2.27	0.47
40:L:79:GLU:OE2	40:L:82:ARG:NH1	2.47	0.47
44:P:30:ARG:HD2	44:P:63:TYR:HE2	1.78	0.47
44:P:114:ILE:HD11	44:P:117:ILE:HB	1.96	0.47
44:P:122:ALA:HB3	44:P:143:PRO:HG2	1.95	0.47
52:X:147:LEU:HD11	87:YY:20:ARG:HH22	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
79:x:126:VAL:HG12	79:x:141:THR:HG22	1.94	0.47
86:XX:68:ILE:HD13	86:XX:68:ILE:N	2.28	0.47
86:XX:254:VAL:O	86:XX:257:TYR:HB3	2.13	0.47
4:DD:164:PRO:HB3	4:DD:170:PRO:HA	1.95	0.47
15:l:248:GLN:O	15:l:253:GLN:CG	2.61	0.47
39:K:641:A:O2'	39:K:645:C:OP1	2.32	0.47
39:K:664:A:O2'	39:K:670:A:N1	2.41	0.47
39:K:903:A:OP1	39:K:903:A:C8	2.67	0.47
52:X:83:THR:HA	86:XX:403:GLY:HA2	1.96	0.47
73:r:85:ASN:N	73:r:85:ASN:OD1	2.44	0.47
76:u:86:LEU:HB3	76:u:98:THR:HB	1.96	0.47
78:w:49:ILE:HG12	78:w:87:TYR:HB2	1.95	0.47
79:x:18:TRP:O	79:x:51:ARG:NH1	2.46	0.47
86:XX:64:TRP:H	86:XX:64:TRP:HD1	1.58	0.47
86:XX:253:ALA:CA	87:YY:33:PHE:CE1	2.97	0.47
86:XX:256:ILE:CD1	87:YY:33:PHE:CD1	2.97	0.47
10:JJ:23:ARG:NH2	10:JJ:29:ASN:OD1	2.38	0.47
19:5:268:G:H2'	19:5:269:G:C8	2.50	0.47
19:5:1558:A:H2'	19:5:1559:G:C8	2.49	0.47
19:5:1867:A:OP1	37:I:13:LYS:NZ	2.41	0.47
30:B:218:ASP:HB2	30:B:348:ARG:HB3	1.96	0.47
39:K:398:A:H5''	39:K:400:C:H5'	1.95	0.47
39:K:444:G:N1	39:K:447:A:OP2	2.46	0.47
48:T:45:MET:H	48:T:95:HIS:HD2	1.63	0.47
79:x:126:VAL:HA	79:x:141:THR:HA	1.95	0.47
19:5:169:A:C3'	19:5:170:C:H5'	2.29	0.47
19:5:1518:A:H61	40:L:19:GLN:HE22	1.61	0.47
19:5:1655:C:OP2	56:a:26:ARG:NH1	2.48	0.47
19:5:1942:A:N3	19:5:4432:C:O2'	2.45	0.47
19:5:2457:G:H21	19:5:3672:G:N2	2.12	0.47
19:5:2583:C:OP2	62:g:76:ARG:NH1	2.44	0.47
26:PP:27:LYS:HG3	26:PP:110:LEU:HD23	1.95	0.47
30:B:303:ALA:HA	30:B:368:ILE:HD12	1.96	0.47
32:D:17:GLN:NE2	48:T:22:HIS:O	2.34	0.47
32:D:108:ARG:CZ	32:D:253:TYR:HB2	2.45	0.47
35:G:119:GLN:HA	35:G:122:ILE:HB	1.96	0.47
39:K:77:A:O2'	81:z:174:PRO:O	2.32	0.47
73:r:10:VAL:HG13	73:r:14:SER:HB3	1.95	0.47
86:XX:20:GLN:O	88:ZZ:68:VAL:C	2.57	0.47
86:XX:72:ASN:CB	86:XX:79:LEU:HD22	2.19	0.47
13:MM:17:LEU:O	76:u:30:TRP:NE1	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1:249:TRP:CZ3	15:1:253:GLN:OE1	2.67	0.47
15:1:251:ARG:HE	19:5:3908:A:H1'	1.78	0.47
16:2:64:U:H2'	16:2:65:C:C6	2.49	0.47
17:3:47:U:O2'	17:3:50:A:OP1	2.30	0.47
19:5:929:A:H3'	19:5:930:G:H8	1.79	0.47
24:NN:52:PRO:HA	24:NN:55:ILE:HD12	1.95	0.47
36:H:20:LEU:HD21	36:H:47:LEU:HB2	1.96	0.47
54:Z:41:ALA:HB2	54:Z:77:TYR:HE1	1.79	0.47
86:XX:34:TRP:CZ3	88:ZZ:74:LEU:HD11	2.50	0.47
86:XX:303:VAL:CG2	86:XX:345:LEU:HD21	2.43	0.47
86:XX:369:LEU:HB3	86:XX:426:LEU:CD1	2.39	0.47
86:XX:375:PHE:O	86:XX:379:TRP:CB	2.62	0.47
5:EE:79:LYS:HB2	5:EE:87:VAL:HB	1.97	0.47
10:JJ:23:ARG:NH1	10:JJ:27:SER:O	2.48	0.47
10:JJ:36:LYS:HB3	10:JJ:43:ILE:HG12	1.97	0.47
19:5:2846:G:O2'	50:V:19:GLY:O	2.32	0.47
37:I:16:PRO:HA	37:I:95:HIS:HD2	1.78	0.47
41:M:129:LYS:HD2	41:M:132:ARG:HH21	1.79	0.47
48:T:63:ARG:NH2	57:b:30:GLU:OE2	2.47	0.47
72:q:30:LEU:HD21	72:q:35:GLU:HG2	1.95	0.47
73:r:63:VAL:HG22	73:r:79:ARG:HG2	1.96	0.47
75:t:114:ARG:NH2	75:t:161:GLU:OE2	2.48	0.47
15:1:248:GLN:O	15:1:249:TRP:O	2.33	0.47
19:5:4980:C:O2	44:P:69:ARG:NH1	2.48	0.47
26:PP:38:LYS:NZ	26:PP:40:ALA:O	2.41	0.47
29:A:102:LEU:HG	29:A:107:MET:HE2	1.94	0.47
39:K:639:C:H2'	39:K:640:A:C8	2.50	0.47
39:K:880:G:H2'	39:K:881:G:C8	2.50	0.47
75:t:106:PHE:HA	75:t:109:ILE:HD12	1.97	0.47
78:w:109:LEU:HD12	78:w:184:ILE:HD11	1.96	0.47
80:y:39:ILE:HG23	80:y:68:ILE:HG21	1.96	0.47
80:y:49:LEU:HB2	83:UU:50:LYS:HE2	1.95	0.47
86:XX:193:TRP:CZ2	87:YY:54:VAL:HG23	2.50	0.47
86:XX:248:THR:N	86:XX:440:ALA:CB	2.38	0.47
19:5:4565:C:OP1	43:O:65:ASN:ND2	2.44	0.47
19:5:4736:C:H2'	19:5:4737:G:C8	2.50	0.47
20:6:251:ALA:HB2	20:6:289:LEU:HD22	1.96	0.47
32:D:64:ILE:HG13	32:D:105:LEU:HD21	1.97	0.47
39:K:907:G:H2'	39:K:908:A:C8	2.50	0.47
43:O:116:LYS:HD3	47:S:169:THR:HG21	1.97	0.47
78:w:29:LEU:HD22	78:w:58:VAL:HG12	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
86:XX:212:ALA:HB3	86:XX:215:ALA:H	1.79	0.47
11:KK:31:ASN:HD21	11:KK:55:THR:HG22	1.79	0.47
12:LL:7:ASN:O	12:LL:9:GLY:N	2.45	0.47
13:MM:137:SER:OG	13:MM:138:ASP:N	2.47	0.47
15:1:251:ARG:CG	15:1:251:ARG:NH1	2.73	0.47
15:1:254:PRO:CG	19:5:4555:U:H2'	2.43	0.47
15:1:256:TRP:O	15:1:256:TRP:HE3	1.97	0.47
19:5:408:A:H4'	19:5:409:G:H3'	1.96	0.47
19:5:1312:A:O2'	60:e:44:ARG:NH2	2.48	0.47
19:5:1986:U:C4	19:5:2013:A:N6	2.83	0.47
19:5:2520:C:H2'	19:5:2521:G:C8	2.50	0.47
19:5:4981:G:H1'	44:P:69:ARG:HD2	1.96	0.47
20:6:88:ARG:HH22	39:K:1398:G:H4'	1.79	0.47
39:K:1407:U:O2'	83:UU:11:GLN:NE2	2.42	0.47
39:K:1588:A:H2'	39:K:1589:A:C8	2.50	0.47
43:O:130:LYS:HB2	43:O:133:ARG:HG2	1.97	0.47
57:b:43:MET:HE2	57:b:43:MET:HB3	1.76	0.47
78:w:126:ILE:HD12	78:w:188:ILE:HG12	1.97	0.47
86:XX:256:ILE:HB	87:YY:36:ILE:HG13	1.95	0.47
15:1:244:PRO:HB2	19:5:1600:A:C2	2.50	0.47
16:2:2:C:C3'	16:2:2:C:H6	2.26	0.47
19:5:1503:A:H4'	19:5:1504:G:H5'	1.97	0.47
19:5:1933:G:H2'	19:5:1934:A:C8	2.50	0.47
19:5:4492:U:O2'	19:5:4512:U:O2	2.31	0.47
25:OO:79:ILE:HB	25:OO:83:LEU:HD12	1.97	0.47
85:WW:52:LYS:HE3	85:WW:80:LEU:HD21	1.96	0.47
86:XX:76:LEU:HD21	86:XX:154:GLN:HE21	1.80	0.47
16:2:61:C:H2'	16:2:62:C:H6	1.80	0.46
19:5:982:U:O2	19:5:1273:G:N2	2.38	0.46
39:K:107:A:H2'	39:K:108:G:C8	2.50	0.46
76:u:129:THR:OG1	76:u:131:ASP:O	2.32	0.46
81:z:78:SER:H	81:z:81:HIS:CD2	2.33	0.46
81:z:181:THR:HG22	81:z:184:VAL:HG23	1.96	0.46
19:5:74:G:H5'	40:L:59:VAL:HG13	1.97	0.46
21:7:11:A:O2'	21:7:13:A:OP2	2.33	0.46
29:A:117:GLU:HG2	29:A:124:GLY:H	1.79	0.46
38:J:27:GLY:HA2	38:J:68:ILE:HG23	1.97	0.46
44:P:131:ARG:HG3	44:P:137:ASN:ND2	2.30	0.46
75:t:15:LEU:HD11	75:t:32:ILE:HD11	1.96	0.46
86:XX:443:SER:CB	86:XX:447:ILE:HD12	2.39	0.46
2:BB:27:LEU:HD23	2:BB:30:LEU:HD12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BB:137:SER:OG	2:BB:162:GLN:O	2.33	0.46
3:CC:10:LYS:HD3	39:K:386:C:H5''	1.97	0.46
16:2:24:A:H2'	16:2:25:C:C6	2.50	0.46
16:2:76:A:C8	16:2:76:A:C3'	2.98	0.46
19:5:1968:G:OP1	74:s:112:ARG:NH1	2.48	0.46
31:C:211:TYR:HE1	31:C:229:LEU:HB3	1.80	0.46
37:I:16:PRO:HA	37:I:95:HIS:CD2	2.51	0.46
54:Z:42:LEU:HD12	54:Z:98:LYS:HG3	1.96	0.46
76:u:103:MET:HE1	76:u:212:VAL:HG23	1.98	0.46
81:z:63:MET:N	81:z:63:MET:SD	2.86	0.46
86:XX:93:LEU:O	86:XX:97:ALA:N	2.43	0.46
86:XX:175:LEU:HD23	86:XX:460:ILE:C	2.40	0.46
3:CC:73:THR:HG23	39:K:302:A:H1'	1.95	0.46
15:1:241:TYR:HD1	15:1:241:TYR:C	2.23	0.46
19:5:2407:G:O6	67:l:2:SER:N	2.49	0.46
19:5:2793:G:C5	19:5:2799:G:N1	2.72	0.46
19:5:3917:A:C8	19:5:3917:A:C5'	2.95	0.46
39:K:369:C:N4	39:K:1731:A:OP1	2.48	0.46
60:e:70:LEU:HD21	60:e:76:LYS:HE2	1.97	0.46
63:h:10:ARG:HH12	63:h:63:GLN:HG3	1.80	0.46
65:j:45:ARG:HH21	65:j:47:TYR:HE2	1.63	0.46
82:TT:52:ILE:HG22	82:TT:61:ILE:HG12	1.98	0.46
86:XX:20:GLN:O	88:ZZ:69:GLY:HA2	2.14	0.46
86:XX:66:ARG:HA	86:XX:66:ARG:NE	2.29	0.46
88:ZZ:79:LEU:HD23	88:ZZ:79:LEU:O	2.14	0.46
1:AA:109:MET:SD	1:AA:113:ARG:NH2	2.87	0.46
3:CC:103:LEU:HD22	3:CC:170:LYS:HB3	1.97	0.46
4:DD:121:LYS:H	4:DD:125:HIS:HD2	1.64	0.46
15:1:259:LEU:CB	19:5:4452:U:H1'	2.45	0.46
19:5:4518:A:OP1	19:5:4520:G:O2'	2.26	0.46
34:F:195:THR:O	34:F:195:THR:OG1	2.33	0.46
39:K:472:C:O2	39:K:475:C:N4	2.46	0.46
49:U:24:ASP:OD1	49:U:24:ASP:N	2.43	0.46
80:y:20:PHE:N	80:y:23:TRP:O	2.45	0.46
86:XX:61:PRO:O	86:XX:65:MET:CA	2.57	0.46
86:XX:177:SER:HG	86:XX:180:SER:H	1.59	0.46
5:EE:126:VAL:HG23	5:EE:145:VAL:HG22	1.96	0.46
10:JJ:68:GLY:O	39:K:928:G:N2	2.42	0.46
16:2:2:C:H2'	16:2:3:U:C6	2.50	0.46
19:5:1481:C:O2'	19:5:1482:G:O5'	2.34	0.46
19:5:2280:G:N2	19:5:2281:U:O4	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:5:4524:G:N3	30:B:252:ALA:HB1	2.31	0.46
30:B:77:THR:HG21	30:B:337:VAL:HG22	1.98	0.46
42:N:116:LEU:HD22	42:N:135:ILE:HD11	1.98	0.46
45:Q:122:THR:OG1	45:Q:124:ASP:OD1	2.28	0.46
52:X:156:ILE:HG12	86:XX:416:TYR:CZ	2.44	0.46
55:SS:5:LYS:NZ	55:SS:82:TYR:OH	2.40	0.46
86:XX:107:LYS:O	86:XX:108:ASP:N	2.44	0.46
1:AA:85:VAL:HA	1:AA:88:GLN:HG2	1.98	0.46
8:HH:32:ILE:HG21	8:HH:34:MET:HG2	1.97	0.46
12:LL:98:PRO:O	39:K:1868:U:N3	2.43	0.46
19:5:1524:A:H61	19:5:1651:G:H22	1.64	0.46
27:QQ:14:SER:HB2	39:K:1016:U:H5''	1.98	0.46
30:B:223:THR:HB	30:B:275:HIS:H	1.81	0.46
32:D:65:ALA:HB2	32:D:74:ILE:HD13	1.96	0.46
39:K:940:U:H3	39:K:1002:U:H3	1.63	0.46
47:S:13:VAL:HG22	47:S:63:TYR:HB3	1.98	0.46
53:Y:26:ARG:NH1	53:Y:75:ARG:O	2.47	0.46
64:i:45:ARG:NH1	64:i:49:GLY:O	2.44	0.46
71:p:14:TYR:O	71:p:17:ARG:NE	2.46	0.46
72:q:122:LEU:HD11	72:q:142:LEU:HD13	1.98	0.46
77:v:113:GLN:HB3	77:v:122:THR:HA	1.98	0.46
4:DD:137:VAL:HG22	4:DD:157:ILE:HG12	1.97	0.46
19:5:1734:G:N2	19:5:1735:U:O4	2.42	0.46
19:5:2422:C:OP1	44:P:127:ARG:NH2	2.48	0.46
19:5:2837:U:OP1	30:B:249:ARG:NH1	2.38	0.46
19:5:2874:U:O2'	19:5:2876:G:N7	2.48	0.46
19:5:4704:C:H4'	36:H:129:ARG:HH22	1.80	0.46
30:B:161:ARG:HG2	30:B:184:GLN:HA	1.98	0.46
81:z:37:ALA:HA	81:z:49:VAL:HA	1.98	0.46
86:XX:59:ALA:HB1	86:XX:65:MET:SD	2.54	0.46
4:DD:113:GLN:OE1	4:DD:154:GLN:NE2	2.49	0.46
9:II:14:ARG:NH2	38:J:114:ASP:OD1	2.49	0.46
16:2:18:G:C2'	16:2:57:G:H22	2.15	0.46
16:2:48:C:N3	16:2:59:A:N7	2.49	0.46
19:5:2341:A:N7	56:a:4:ARG:NH2	2.64	0.46
19:5:3736:A:H2'	19:5:3737:A:C8	2.51	0.46
19:5:4448:G:H5''	19:5:4449:A:H5'	1.98	0.46
19:5:4537:C:H2'	19:5:4538:G:C8	2.51	0.46
21:7:7:G:OP1	32:D:33:ARG:NE	2.36	0.46
25:OO:47:LEU:HB2	25:OO:79:ILE:HG22	1.98	0.46
39:K:367:U:H4'	39:K:371:A:C8	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:Q:184:ARG:NE	56:a:55:LYS:O	2.49	0.46
54:Z:61:LYS:O	54:Z:65:ARG:HB2	2.15	0.46
63:h:38:GLY:O	86:XX:266:PRO:HD3	2.15	0.46
73:r:17:LEU:HD21	73:r:19:LYS:HE3	1.97	0.46
81:z:2:LYS:HB2	81:z:108:VAL:HG22	1.98	0.46
83:UU:16:LYS:HG3	83:UU:17:LYS:H	1.81	0.46
86:XX:11:PRO:CA	86:XX:111:LEU:HD13	2.45	0.46
86:XX:188:CYS:SG	87:YY:44:PHE:CA	3.02	0.46
86:XX:302:TYR:HD2	86:XX:345:LEU:CD2	2.28	0.46
86:XX:394:LEU:HD23	86:XX:394:LEU:HA	1.78	0.46
88:ZZ:71:VAL:O	88:ZZ:75:VAL:HG23	2.15	0.46
11:KK:28:PHE:HA	11:KK:55:THR:HG21	1.98	0.46
15:1:257:LYS:HB2	15:1:257:LYS:HE3	1.40	0.46
16:2:75:C:N3	19:5:4196:G:O6	2.49	0.46
19:5:369:G:N2	19:5:372:A:OP2	2.44	0.46
19:5:2566:G:H2'	19:5:2567:G:H8	1.81	0.46
20:6:35:SER:OG	20:6:37:ASP:OD1	2.30	0.46
20:6:87:LEU:HB2	20:6:101:PHE:HB2	1.98	0.46
29:A:179:ILE:HG23	29:A:184:ARG:HB2	1.98	0.46
39:K:903:A:P	39:K:903:A:O4'	2.74	0.46
72:q:33:GLN:HB3	72:q:154:LEU:HD12	1.96	0.46
80:y:39:ILE:HG23	80:y:68:ILE:HD13	1.98	0.46
86:XX:115:ALA:HA	86:XX:118:LEU:HD12	1.97	0.46
2:BB:133:LEU:HD11	2:BB:177:TYR:HB2	1.98	0.45
19:5:66:A:O2'	19:5:326:C:O2	2.32	0.45
19:5:970:G:OP1	19:5:2259:G:N2	2.46	0.45
19:5:4370:G:H5''	70:o:64:LYS:HG3	1.97	0.45
20:6:110:SER:OG	20:6:155:ARG:NH1	2.44	0.45
35:G:313:GLU:O	35:G:317:LYS:NZ	2.36	0.45
39:K:1232:U:H2'	39:K:1233:G:C8	2.51	0.45
54:Z:105:ALA:HA	54:Z:108:ARG:HE	1.81	0.45
72:q:181:GLU:OE2	72:q:191:ARG:NH2	2.42	0.45
86:XX:34:TRP:HH2	88:ZZ:71:VAL:CG2	2.29	0.45
86:XX:155:LEU:O	86:XX:159:GLY:N	2.49	0.45
3:CC:162:LEU:HD11	3:CC:191:GLU:HG2	1.98	0.45
19:5:1368:A:H1'	53:Y:1:MET:HE2	1.97	0.45
19:5:3932:U:H2'	19:5:3933:G:C8	2.51	0.45
19:5:4398:C:C6	19:5:4398:C:C4'	2.99	0.45
25:OO:68:ILE:HB	25:OO:109:TYR:HB2	1.98	0.45
39:K:1272:C:O2'	39:K:1274:G:N2	2.50	0.45
43:O:55:LEU:HD23	43:O:58:LEU:HD12	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:R:4:LEU:HD11	46:R:29:THR:HG23	1.99	0.45
82:TT:15:ASN:HD21	82:TT:71:LYS:HG3	1.80	0.45
84:VV:72:VAL:N	84:VV:81:ILE:O	2.39	0.45
86:XX:259:GLN:HG2	86:XX:284:PHE:HE2	1.73	0.45
3:CC:25:ARG:HA	39:K:448:A:H5''	1.97	0.45
12:LL:92:ARG:HB3	39:K:1865:C:O2	2.16	0.45
19:5:952:G:H5''	61:f:73:LYS:HD3	1.97	0.45
19:5:2777:G:H5''	19:5:2778:G:H5'	1.98	0.45
19:5:4249:G:O2'	38:J:98:ASN:O	2.32	0.45
19:5:4389:C:H2'	19:5:4390:A:H8	1.82	0.45
30:B:53:MET:SD	30:B:77:THR:HG22	2.56	0.45
39:K:454:U:H5''	81:z:94:ARG:HG2	1.98	0.45
39:K:928:G:H2'	39:K:929:G:C8	2.52	0.45
50:V:82:ILE:HG22	50:V:83:ARG:HG3	1.97	0.45
75:t:141:CYS:SG	75:t:142:ASN:N	2.89	0.45
86:XX:35:THR:OG1	86:XX:36:ALA:N	2.50	0.45
86:XX:38:THR:HG21	86:XX:169:LEU:HD11	1.99	0.45
86:XX:198:PRO:HG3	87:YY:55:LYS:HD2	1.98	0.45
19:5:909:G:H2'	19:5:910:G:H8	1.80	0.45
19:5:1942:A:H2'	19:5:1943:A:C8	2.51	0.45
19:5:1951:G:O2'	47:S:95:ARG:NH2	2.35	0.45
19:5:2627:C:H41	19:5:4649:G:H1	1.65	0.45
39:K:31:U:O2'	39:K:643:A:N1	2.45	0.45
43:O:27:VAL:HG12	43:O:98:ALA:HB1	1.98	0.45
48:T:143:THR:OG1	48:T:146:LYS:O	2.33	0.45
53:Y:13:LYS:O	53:Y:17:ARG:HG2	2.16	0.45
58:c:11:LEU:HD23	58:c:14:ILE:HD12	1.97	0.45
63:h:67:GLU:HA	63:h:70:ARG:HG2	1.99	0.45
86:XX:168:LEU:HD11	88:ZZ:73:VAL:HG11	1.98	0.45
86:XX:401:MET:H	86:XX:409:MET:HE2	1.80	0.45
19:5:1656:U:O2'	19:5:3906:A:N1	2.36	0.45
19:5:2400:G:H21	62:g:6:THR:HG22	1.82	0.45
19:5:2404:A:OP2	67:l:2:SER:OG	2.34	0.45
19:5:2674:A:N6	58:c:51:ASN:O	2.50	0.45
23:9:8:TRP:HZ3	39:K:1512:C:H5''	1.81	0.45
24:NN:15:ASN:HB2	24:NN:20:ARG:HG2	1.97	0.45
30:B:314:ILE:H	30:B:314:ILE:HG13	1.59	0.45
32:D:208:MET:HB2	32:D:208:MET:HE3	1.66	0.45
39:K:1674:G:OP1	80:y:51:HIS:NE2	2.37	0.45
41:M:119:ARG:HH21	41:M:123:ILE:HD11	1.82	0.45
52:X:89:LYS:HD3	52:X:93:ASN:HD22	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
74:s:194:ASP:O	74:s:197:SER:OG	2.31	0.45
86:XX:188:CYS:O	87:YY:44:PHE:CZ	2.70	0.45
86:XX:248:THR:O	86:XX:251:VAL:CG2	2.64	0.45
86:XX:306:GLN:O	86:XX:309:SER:OG	2.35	0.45
86:XX:441:ILE:CG1	86:XX:444:GLY:N	2.80	0.45
16:2:2:C:C6	16:2:2:C:O5'	2.70	0.45
19:5:1375:C:OP1	31:C:274:LYS:NZ	2.40	0.45
19:5:1497:A:H1'	45:Q:164:LYS:HG3	1.98	0.45
19:5:3653:A:O2'	29:A:179:ILE:O	2.33	0.45
19:5:3788:C:N4	19:5:3812:C:OP2	2.45	0.45
19:5:4078:C:O2'	19:5:4172:A:N6	2.50	0.45
19:5:4925:U:H4'	19:5:4926:C:H5'	1.99	0.45
20:6:146:SER:OG	20:6:147:HIS:N	2.50	0.45
31:C:339:THR:HA	31:C:342:ARG:HB3	1.98	0.45
39:K:346:C:H5''	79:x:38:LEU:HB2	1.98	0.45
41:M:119:ARG:HH11	43:O:202:LEU:HD21	1.82	0.45
51:W:116:LYS:HE3	51:W:120:GLN:HE21	1.82	0.45
73:r:6:GLN:HG3	73:r:44:ILE:HG12	1.99	0.45
74:s:145:THR:HG22	74:s:154:ILE:HG13	1.98	0.45
77:v:264:SER:O	77:v:268:GLU:N	2.43	0.45
4:DD:114:VAL:HG12	4:DD:120:ALA:HB2	1.98	0.45
11:KK:111:PHE:HB3	11:KK:114:LEU:HD21	1.99	0.45
17:3:75:C:O2'	70:o:54:PRO:O	2.27	0.45
19:5:12:A:H5''	19:5:12:A:H8	1.81	0.45
21:7:47:G:H21	32:D:222:GLN:HE22	1.65	0.45
29:A:80:GLU:HG3	71:p:66:GLY:HA2	1.98	0.45
39:K:941:C:H2'	39:K:942:G:C8	2.52	0.45
39:K:1553:C:O2'	39:K:1554:C:O4'	2.34	0.45
41:M:49:ALA:HB2	47:S:100:LEU:HD11	1.99	0.45
44:P:29:THR:HA	44:P:32:THR:HG22	1.98	0.45
46:R:115:ILE:HG22	46:R:119:MET:HE3	1.99	0.45
47:S:14:GLY:HA2	47:S:62:VAL:HG23	1.99	0.45
52:X:147:LEU:HG	87:YY:20:ARG:HH22	1.81	0.45
78:w:59:LEU:HA	78:w:66:ILE:HG13	1.99	0.45
83:UU:89:SER:HB2	83:UU:112:LEU:HD13	1.98	0.45
8:HH:64:GLU:OE2	72:q:33:GLN:NE2	2.38	0.45
26:PP:11:GLN:OE1	26:PP:62:ARG:NH1	2.44	0.45
47:S:13:VAL:HG23	47:S:62:VAL:HB	1.99	0.45
52:X:156:ILE:HD11	86:XX:415:ARG:HH11	1.80	0.45
58:c:61:GLU:OE2	58:c:73:HIS:NE2	2.37	0.45
62:g:68:SER:HB3	62:g:71:LYS:HD3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
64:i:90:LEU:HA	64:i:93:VAL:HG22	1.99	0.45
72:q:60:LEU:HD22	72:q:159:ILE:HG12	1.99	0.45
81:z:93:LYS:HD2	81:z:95:LYS:HE2	1.99	0.45
85:WW:56:LEU:HD22	85:WW:80:LEU:HD12	1.98	0.45
85:WW:75:VAL:HG21	85:WW:104:GLN:HE22	1.82	0.45
86:XX:66:ARG:NH1	86:XX:79:LEU:CA	2.80	0.45
86:XX:376:SER:OG	86:XX:377:LYS:N	2.50	0.45
16:2:76:A:C8	16:2:76:A:C4'	3.00	0.45
19:5:280:G:OP2	42:N:44:ARG:NH2	2.50	0.45
19:5:2380:G:N2	19:5:2424:G:H5'	2.32	0.45
19:5:2422:C:O2'	19:5:3857:G:O2'	2.34	0.45
19:5:3707:U:H2'	19:5:3708:C:C6	2.52	0.45
19:5:4762:A:H62	47:S:171:ARG:HB2	1.82	0.45
26:PP:121:ARG:NH2	39:K:1563:G:OP1	2.50	0.45
29:A:48:ILE:HD11	29:A:82:ILE:HG22	1.98	0.45
39:K:1562:C:H2'	39:K:1563:G:H8	1.82	0.45
43:O:121:PRO:HD3	47:S:168:THR:HG22	1.99	0.45
50:V:13:LYS:NZ	50:V:57:VAL:O	2.39	0.45
50:V:21:PRO:HA	50:V:54:ALA:HA	1.98	0.45
52:X:147:LEU:HG	87:YY:20:ARG:HH12	1.82	0.45
82:TT:102:ILE:H	82:TT:113:HIS:CD2	2.34	0.45
86:XX:441:ILE:CD1	86:XX:444:GLY:N	2.78	0.45
3:CC:7:ASN:HD22	39:K:386:C:H5'	1.82	0.45
9:II:34:LYS:HB2	9:II:100:ALA:HA	1.99	0.45
19:5:89:C:OP1	56:a:59:ARG:NH1	2.50	0.45
26:PP:56:ARG:HH22	26:PP:99:VAL:HB	1.82	0.45
31:C:328:LEU:HD22	34:F:186:MET:HE2	1.99	0.45
32:D:54:ARG:HB3	38:J:146:ARG:HH12	1.82	0.45
36:H:41:ILE:HG12	36:H:73:ILE:HD11	1.99	0.45
63:h:28:LEU:HD21	63:h:32:ARG:HE	1.82	0.45
86:XX:66:ARG:HH21	86:XX:70:ALA:CA	2.01	0.45
15:1:246:LEU:HD13	19:5:1600:A:N3	2.32	0.44
19:5:115:C:O2'	19:5:276:C:OP1	2.32	0.44
19:5:978:G:H21	19:5:1277:G:H1	1.65	0.44
19:5:1949:U:OP1	36:H:64:ARG:NH1	2.50	0.44
19:5:2015:U:H2'	19:5:2016:C:H6	1.82	0.44
19:5:2779:C:H5'	52:X:105:ASN:HD22	1.81	0.44
19:5:4122:G:O3'	62:g:90:ARG:NH1	2.50	0.44
19:5:4478:G:O2'	19:5:4602:A:N1	2.47	0.44
19:5:4611:A:H2	36:H:120:GLU:HG2	1.81	0.44
33:E:165:VAL:HG13	33:E:180:GLY:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:K:220:U:H2'	39:K:221:A:C8	2.53	0.44
50:V:112:MET:HE2	50:V:112:MET:HB3	1.84	0.44
54:Z:27:LYS:NZ	54:Z:97:ASN:OD1	2.49	0.44
79:x:207:VAL:HA	79:x:221:ARG:HA	1.98	0.44
19:5:93:G:OP2	56:a:54:GLY:N	2.50	0.44
19:5:2622:G:O6	49:U:81:ARG:NH2	2.48	0.44
33:E:206:ILE:HD11	33:E:260:ILE:HG12	2.00	0.44
37:I:79:SER:OG	37:I:147:HIS:ND1	2.51	0.44
39:K:1221:G:O2'	39:K:1676:U:O2	2.29	0.44
45:Q:85:THR:HG22	45:Q:104:ARG:HB3	1.99	0.44
45:Q:179:GLY:H	56:a:51:GLY:H	1.65	0.44
47:S:127:MET:HE1	48:T:155:PRO:HA	2.00	0.44
73:r:18:ILE:HG23	73:r:25:TYR:HB2	1.98	0.44
78:w:46:THR:HB	78:w:84:VAL:HA	1.99	0.44
79:x:44:LEU:HD13	79:x:72:ILE:HD11	1.98	0.44
79:x:137:PRO:HB2	79:x:150:PRO:HD2	1.98	0.44
3:CC:45:THR:HG22	39:K:307:G:H1'	1.98	0.44
7:GG:67:LYS:HB3	39:K:1337:C:H4'	1.99	0.44
19:5:2638:G:H1	19:5:2697:A:H61	1.64	0.44
19:5:3915:U:H2'	19:5:3916:G:H5''	2.00	0.44
39:K:65:C:C4	81:z:133:LEU:HD23	2.52	0.44
40:L:153:PRO:HG2	40:L:156:PRO:HB3	1.99	0.44
76:u:131:ASP:OD1	76:u:131:ASP:N	2.49	0.44
86:XX:196:PHE:H	87:YY:52:PHE:HZ	1.65	0.44
3:CC:83:TYR:HB3	3:CC:101:ILE:HB	1.99	0.44
19:5:152:U:P	42:N:49:ARG:HH12	2.41	0.44
19:5:1328:G:O2'	19:5:2349:A:OP1	2.34	0.44
19:5:1516:G:OP2	56:a:32:ARG:NH1	2.51	0.44
19:5:3812:C:H3'	19:5:3813:A:H2'	1.99	0.44
25:OO:48:VAL:HG22	25:OO:80:ARG:HE	1.82	0.44
31:C:28:PHE:HA	31:C:129:ALA:HA	1.99	0.44
35:G:225:ALA:HB3	64:i:43:MET:HE1	1.99	0.44
39:K:1010:G:H2'	39:K:1011:A:C8	2.53	0.44
39:K:1277:C:H2'	39:K:1278:A:H8	1.83	0.44
43:O:54:TYR:OH	43:O:73:PHE:O	2.34	0.44
60:e:113:GLU:OE2	60:e:117:GLN:NE2	2.49	0.44
63:h:38:GLY:HA3	86:XX:266:PRO:CB	2.35	0.44
70:o:6:LYS:HG2	70:o:93:LEU:HB3	1.99	0.44
77:v:137:VAL:HG21	77:v:244:ILE:HD12	1.99	0.44
86:XX:61:PRO:O	86:XX:65:MET:N	2.51	0.44
1:AA:104:ARG:HB3	4:DD:38:ARG:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:CC:49:ARG:HE	39:K:446:G:H5''	1.81	0.44
15:1:256:TRP:O	15:1:256:TRP:CE3	2.70	0.44
19:5:1590:C:H4'	19:5:2857:A:H5'	1.99	0.44
19:5:1638:A:C5	65:j:8:PHE:CE2	3.05	0.44
19:5:3777:G:O2'	19:5:3815:G:O6	2.34	0.44
25:OO:47:LEU:H	25:OO:79:ILE:HA	1.82	0.44
33:E:115:MET:O	73:r:87:ARG:NH1	2.46	0.44
35:G:101:LYS:HD2	52:X:42:THR:HG23	1.98	0.44
37:I:36:LEU:HD11	37:I:87:ILE:HD12	1.98	0.44
39:K:798:G:C8	39:K:798:G:H5''	2.53	0.44
39:K:1397:U:H5''	39:K:1398:G:H8	1.82	0.44
46:R:148:ASP:OD1	46:R:151:ARG:NH2	2.44	0.44
51:W:9:SER:OG	51:W:36:CYS:SG	2.75	0.44
70:o:63:THR:OG1	70:o:88:CYS:O	2.35	0.44
86:XX:450:ALA:HA	86:XX:453:ILE:HD12	2.00	0.44
87:YY:32:GLU:CD	87:YY:32:GLU:N	2.73	0.44
14:O:105:TYR:HB3	14:O:131:PHE:HE2	1.83	0.44
16:2:53:G:H2'	16:2:54:U:H6	1.81	0.44
19:5:2318:G:N2	19:5:2321:G:OP2	2.44	0.44
19:5:4125:C:H4'	35:G:98:ILE:HG21	1.99	0.44
23:9:34:TYR:OH	39:K:1549:U:OP1	2.33	0.44
29:A:112:ILE:HG13	71:p:79:VAL:HG22	1.98	0.44
29:A:115:CYS:HA	29:A:128:ARG:HB3	2.00	0.44
30:B:215:GLU:OE2	30:B:349:LYS:NZ	2.42	0.44
39:K:528:A:H2'	39:K:529:A:H8	1.82	0.44
48:T:45:MET:H	48:T:95:HIS:CD2	2.36	0.44
52:X:104:ALA:O	52:X:134:LYS:NZ	2.50	0.44
53:Y:52:ASP:HB2	53:Y:110:LYS:HG3	1.98	0.44
86:XX:121:MET:HE3	86:XX:156:PHE:HD1	1.81	0.44
86:XX:188:CYS:HG	87:YY:44:PHE:HA	1.80	0.44
86:XX:285:TYR:O	86:XX:285:TYR:CD2	2.70	0.44
86:XX:376:SER:O	86:XX:379:TRP:N	2.47	0.44
15:1:241:TYR:C	15:1:241:TYR:CD1	2.94	0.44
16:2:2:C:C5	16:2:2:C:OP2	2.70	0.44
19:5:2411:C:H2'	19:5:2412:A:C8	2.52	0.44
19:5:3680:U:OP1	29:A:54:ARG:NH2	2.51	0.44
19:5:4594:U:H2'	19:5:4595:G:H8	1.82	0.44
19:5:4927:G:OP2	19:5:4927:G:N2	2.41	0.44
29:A:225:ILE:HD11	29:A:233:ARG:HG3	1.98	0.44
39:K:223:C:H2'	39:K:224:A:C8	2.52	0.44
39:K:1743:G:H21	39:K:1791:A:H62	1.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:M:89:THR:HG22	41:M:91:TRP:H	1.82	0.44
86:XX:302:TYR:HE2	86:XX:341:LEU:HB3	1.82	0.44
86:XX:443:SER:CB	86:XX:447:ILE:HG13	2.31	0.44
8:HH:1:MET:SD	8:HH:1:MET:N	2.86	0.44
10:JJ:2:PRO:HG2	10:JJ:5:LYS:HD2	2.00	0.44
19:5:1823:G:O2'	32:D:44:TYR:O	2.35	0.44
30:B:50:LYS:HB2	30:B:345:LEU:HD22	2.00	0.44
32:D:22:ARG:HH21	32:D:27:LYS:HB3	1.81	0.44
39:K:804:U:OP1	82:TT:82:GLN:NE2	2.51	0.44
47:S:13:VAL:HG12	47:S:29:ARG:HG3	2.00	0.44
52:X:156:ILE:HD12	86:XX:415:ARG:HH12	1.81	0.44
58:c:34:SER:HB2	58:c:95:SER:HB3	1.99	0.44
63:h:37:THR:O	86:XX:266:PRO:HG3	2.18	0.44
74:s:14:PHE:HA	74:s:17:ILE:HG22	2.00	0.44
78:w:50:ILE:HD11	78:w:86:LEU:HD23	2.00	0.44
2:BB:130:LEU:HD23	2:BB:142:LYS:HE2	1.99	0.44
19:5:313:U:H5''	42:N:179:LYS:HE3	1.99	0.44
19:5:734:G:H1	19:5:929:A:H62	1.65	0.44
19:5:4274:A:H2'	19:5:4275:G:C8	2.52	0.44
20:6:254:PRO:HA	20:6:285:GLN:HA	2.00	0.44
26:PP:104:LEU:HD13	26:PP:121:ARG:HG3	1.99	0.44
35:G:130:PRO:HG2	35:G:133:ILE:HD12	2.00	0.44
39:K:494:C:N4	39:K:509:G:H21	2.16	0.44
42:N:178:HIS:HA	42:N:181:HIS:NE2	2.33	0.44
61:f:28:LEU:HD21	61:f:101:ILE:HD11	1.99	0.44
75:t:17:CYS:SG	75:t:18:THR:N	2.91	0.44
86:XX:61:PRO:O	86:XX:65:MET:HE3	1.96	0.44
86:XX:121:MET:HE1	86:XX:160:LEU:HG	1.90	0.44
86:XX:185:THR:HA	87:YY:47:MET:CG	2.48	0.44
86:XX:262:ARG:HG2	87:YY:26:THR:CG2	2.47	0.44
4:DD:60:LEU:HD11	4:DD:73:GLU:HG3	2.00	0.43
21:7:63:C:H5'	21:7:64:G:H5''	2.00	0.43
39:K:197:U:O2	39:K:202:G:O6	2.36	0.43
39:K:854:A:H2'	39:K:855:G:H8	1.83	0.43
39:K:1612:G:OP1	85:WW:18:ARG:NH2	2.51	0.43
82:TT:6:VAL:HG12	82:TT:34:ILE:HD11	1.99	0.43
84:VV:123:VAL:HG12	84:VV:124:LYS:HG3	2.00	0.43
86:XX:10:LYS:O	86:XX:111:LEU:HD22	2.18	0.43
86:XX:61:PRO:HB2	86:XX:65:MET:HB3	1.99	0.43
86:XX:77:MET:C	86:XX:78:GLU:N	2.76	0.43
86:XX:294:GLN:HB3	86:XX:375:PHE:CE2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:5:453:G:O2'	19:5:705:G:OP1	2.32	0.43
19:5:2717:G:OP1	49:U:107:LYS:NZ	2.46	0.43
19:5:4301:U:H4'	48:T:54:HIS:CD2	2.53	0.43
27:QQ:64:ARG:NH2	39:K:919:A:OP2	2.50	0.43
32:D:157:ASN:HD22	32:D:158:LYS:H	1.66	0.43
37:I:135:ILE:HG22	37:I:136:MET:HG3	1.99	0.43
39:K:508:A:H3'	39:K:509:G:H8	1.83	0.43
39:K:1444:U:O2'	39:K:1580:A:N1	2.50	0.43
41:M:47:ARG:HG3	47:S:73:LEU:HD22	1.99	0.43
41:M:47:ARG:HH22	41:M:69:ARG:HA	1.83	0.43
52:X:147:LEU:CD1	87:YY:20:ARG:HH22	2.30	0.43
86:XX:121:MET:HE1	86:XX:156:PHE:O	2.18	0.43
15:1:246:LEU:CD2	15:1:246:LEU:H	2.30	0.43
19:5:4309:G:H5'	19:5:4338:G:H5''	2.00	0.43
36:H:43:VAL:HG12	36:H:59:LYS:HD3	1.99	0.43
39:K:1172:U:H2'	39:K:1173:A:H8	1.83	0.43
53:Y:111:LEU:HD23	53:Y:115:ARG:HG3	2.00	0.43
86:XX:253:ALA:CA	87:YY:33:PHE:CZ	3.01	0.43
86:XX:291:ILE:HG22	86:XX:372:CYS:CB	2.48	0.43
86:XX:461:PHE:O	86:XX:461:PHE:CD1	2.71	0.43
87:YY:33:PHE:O	87:YY:37:ALA:CB	2.66	0.43
88:ZZ:83:SER:O	88:ZZ:87:LEU:CB	2.65	0.43
9:II:39:ARG:HG2	39:K:1629:C:H5''	2.01	0.43
13:MM:67:ASP:OD1	13:MM:67:ASP:N	2.51	0.43
19:5:979:C:H2'	19:5:980:U:C6	2.53	0.43
19:5:4162:C:H5	35:G:126:ARG:HH12	1.66	0.43
34:F:65:ARG:HD3	34:F:65:ARG:HA	1.81	0.43
39:K:1597:C:H4'	39:K:1603:G:C6	2.53	0.43
83:UU:35:ASN:HD21	83:UU:72:VAL:HB	1.83	0.43
86:XX:19:ILE:CB	88:ZZ:69:GLY:H	2.16	0.43
86:XX:188:CYS:CB	87:YY:44:PHE:O	2.66	0.43
86:XX:306:GLN:OE1	86:XX:338:VAL:CG1	2.66	0.43
13:MM:56:VAL:HG11	13:MM:80:ASP:HB3	1.99	0.43
14:O:137:ASP:OD1	14:O:137:ASP:N	2.52	0.43
19:5:1512:G:OP1	56:a:7:LYS:NZ	2.46	0.43
19:5:2409:U:H5	19:5:2783:A:N1	2.16	0.43
19:5:2573:A:H62	19:5:2761:U:H3	1.65	0.43
19:5:4510:A:O2'	19:5:4511:A:O4'	2.36	0.43
39:K:65:C:N4	81:z:134:GLY:O	2.34	0.43
39:K:183:G:O2'	39:K:184:G:O4'	2.32	0.43
39:K:792:C:H2'	39:K:793:G:C8	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:K:798:G:C5'	39:K:798:G:H8	2.31	0.43
42:N:114:ARG:NH1	42:N:153:LYS:O	2.48	0.43
43:O:119:VAL:HG11	47:S:171:ARG:HD3	1.99	0.43
52:X:77:ILE:HD12	52:X:116:LEU:HD12	2.01	0.43
86:XX:69:LEU:HD12	86:XX:69:LEU:HA	1.65	0.43
86:XX:442:GLY:C	86:XX:447:ILE:HD11	2.44	0.43
5:EE:113:LEU:HD23	5:EE:142:VAL:HG21	1.99	0.43
7:GG:40:ILE:HD11	7:GG:53:PRO:HD3	2.01	0.43
13:MM:94:HIS:HD2	13:MM:128:ARG:H	1.66	0.43
16:2:21:A:N1	16:2:46:G:C2	2.85	0.43
19:5:1872:G:O2'	19:5:4219:A:N3	2.46	0.43
19:5:3663:A:OP1	29:A:119:LYS:NZ	2.43	0.43
39:K:125:C:OP1	39:K:127:C:N4	2.46	0.43
39:K:1533:A:O2'	80:y:81:ARG:NH2	2.52	0.43
39:K:1705:C:H2'	39:K:1706:G:C8	2.54	0.43
45:Q:50:ARG:HG2	45:Q:53:MET:HE2	2.01	0.43
56:a:98:ALA:HB2	56:a:121:PRO:HB2	1.98	0.43
72:q:159:ILE:HD12	72:q:159:ILE:HA	1.89	0.43
86:XX:241:ASN:HB3	86:XX:244:ASN:HB2	2.01	0.43
19:5:8:U:H5''	42:N:40:PRO:HG3	2.00	0.43
19:5:172:C:O2	63:h:112:ARG:NH2	2.52	0.43
29:A:242:ARG:NH1	29:A:245:ARG:O	2.52	0.43
31:C:336:ARG:O	31:C:340:ILE:HG12	2.18	0.43
53:Y:49:ILE:HD13	53:Y:80:ILE:HD13	2.01	0.43
59:d:20:VAL:HG12	59:d:91:LYS:HA	1.99	0.43
60:e:86:GLU:HG3	60:e:118:LEU:HD11	2.01	0.43
74:s:29:ILE:HG22	74:s:190:GLN:HB3	2.01	0.43
75:t:76:SER:OG	75:t:77:ALA:N	2.51	0.43
76:u:71:LEU:HD11	76:u:189:ILE:HA	2.00	0.43
84:VV:50:ILE:HG13	84:VV:75:ILE:HD11	1.99	0.43
84:VV:84:PHE:HB2	84:VV:118:VAL:HG11	2.01	0.43
86:XX:193:TRP:HZ2	87:YY:54:VAL:CG2	2.31	0.43
19:5:4327:C:OP1	48:T:70:HIS:NE2	2.51	0.43
19:5:4943:A:OP1	33:E:157:THR:OG1	2.28	0.43
29:A:209:HIS:CE1	29:A:235:VAL:HG11	2.53	0.43
37:I:43:VAL:O	37:I:171:TRP:NE1	2.34	0.43
37:I:191:ILE:HD11	37:I:212:LEU:HD11	2.01	0.43
39:K:1473:G:O2'	39:K:1475:G:N2	2.51	0.43
40:L:164:GLU:HG3	56:a:100:ILE:HB	1.98	0.43
41:M:31:ILE:HG22	41:M:32:ASP:HB2	2.01	0.43
46:R:11:ALA:HB1	46:R:50:ILE:HD13	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
71:p:57:CYS:SG	71:p:59:SER:OG	2.76	0.43
74:s:59:THR:HA	74:s:62:ARG:HD2	2.00	0.43
81:z:67:VAL:HG13	81:z:99:GLY:HA2	2.00	0.43
86:XX:196:PHE:O	87:YY:52:PHE:HE1	2.02	0.43
11:KK:16:ILE:HG22	11:KK:24:LEU:HD11	2.01	0.43
16:2:45:G:O5'	16:2:45:G:C8	2.72	0.43
19:5:1786:A:H2'	19:5:1789:C:C5	2.54	0.43
22:8:38:U:H5'	63:h:81:LEU:HD13	2.01	0.43
39:K:1388:A:H61	78:w:161:GLY:HA3	1.83	0.43
43:O:61:ARG:HD2	43:O:66:PRO:HB3	2.01	0.43
78:w:29:LEU:HD23	78:w:65:ARG:HH22	1.84	0.43
86:XX:6:LEU:CG	86:XX:101:GLU:OE2	2.67	0.43
86:XX:236:ARG:H	86:XX:241:ASN:ND2	2.17	0.43
16:2:24:A:H2'	16:2:25:C:H6	1.84	0.43
16:2:76:A:C8	16:2:76:A:H3'	2.54	0.43
19:5:981:C:H42	19:5:1274:A:H61	1.65	0.43
19:5:1444:G:H21	19:5:2110:G:H1	1.65	0.43
32:D:157:ASN:HD22	32:D:158:LYS:N	2.17	0.43
57:b:36:ASP:HA	57:b:37:PRO:HD3	1.90	0.43
62:g:105:LYS:HB2	62:g:105:LYS:HE3	1.83	0.43
67:l:44:TRP:O	67:l:48:LYS:NZ	2.50	0.43
76:u:68:GLU:HG3	76:u:83:LYS:HD2	2.01	0.43
78:w:142:LEU:HD21	78:w:182:LEU:HD21	1.99	0.43
86:XX:58:SER:HA	86:XX:73:ARG:HE	1.83	0.43
13:MM:147:ARG:NH2	39:K:1854:U:OP2	2.51	0.42
19:5:4277:G:H5''	48:T:17:ARG:HG2	2.01	0.42
20:6:163:PRO:HB2	20:6:179:LEU:HB2	2.01	0.42
32:D:67:ALA:HA	32:D:72:ASP:HB3	2.01	0.42
37:I:17:TYR:H	37:I:95:HIS:CD2	2.35	0.42
39:K:382:C:H2'	39:K:383:G:H8	1.83	0.42
86:XX:161:ILE:HD11	88:ZZ:80:PHE:HB3	2.00	0.42
14:0:100:LEU:HD11	39:K:1285:G:H1'	2.00	0.42
16:2:18:G:N2	16:2:57:G:H2'	2.34	0.42
19:5:189:G:H2'	19:5:190:G:H8	1.84	0.42
19:5:651:C:H2'	19:5:652:G:H8	1.84	0.42
19:5:976:G:H5''	34:F:46:ARG:NH1	2.34	0.42
19:5:1414:C:H2'	19:5:1415:G:H8	1.84	0.42
20:6:120:ILE:O	20:6:132:TRP:N	2.51	0.42
20:6:162:ASN:HB3	20:6:164:ILE:HD12	2.00	0.42
30:B:137:TRP:O	30:B:143:LYS:NZ	2.42	0.42
39:K:878:G:C6	39:K:908:A:N1	2.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:K:1156:U:OP1	82:TT:71:LYS:NZ	2.44	0.42
39:K:1408:U:H2'	39:K:1409:A:C8	2.54	0.42
44:P:36:ILE:HD11	44:P:44:ALA:HB1	2.00	0.42
48:T:31:MET:HB2	48:T:31:MET:HE3	1.62	0.42
79:x:17:HIS:HB2	79:x:108:ARG:HA	2.01	0.42
86:XX:59:ALA:CB	86:XX:79:LEU:HD13	2.49	0.42
86:XX:185:THR:HA	87:YY:47:MET:HB2	1.96	0.42
2:BB:66:VAL:HG22	2:BB:96:ALA:HB1	2.01	0.42
2:BB:103:LYS:H	39:K:688:U:H5	1.66	0.42
14:O:138:ARG:NH1	39:K:1293:A:H1'	2.34	0.42
15:1:249:TRP:CZ3	19:5:3904:G:N2	2.81	0.42
15:1:257:LYS:O	19:5:4451:G:N3	2.52	0.42
15:1:258:PRO:HB2	15:1:259:LEU:HD22	2.02	0.42
19:5:942:G:H5''	34:F:145:ASN:HD21	1.84	0.42
19:5:1795:A:O2'	21:7:97:G:N2	2.52	0.42
20:6:277:THR:HB	20:6:281:ALA:HB3	2.01	0.42
30:B:10:ARG:NH1	30:B:12:GLY:O	2.52	0.42
32:D:286:SER:HA	32:D:289:ARG:HG2	2.00	0.42
33:E:261:LEU:HA	33:E:264:ILE:HG12	2.00	0.42
34:F:89:ALA:HB2	34:F:124:LEU:HD21	2.02	0.42
39:K:1025:U:O3'	39:K:1089:G:N2	2.52	0.42
39:K:1405:A:H2'	39:K:1406:G:O4'	2.19	0.42
39:K:1648:G:O2'	39:K:1674:G:O6	2.35	0.42
61:f:72:GLY:HA2	61:f:88:PHE:HA	2.00	0.42
86:XX:188:CYS:HB2	87:YY:47:MET:HB2	2.01	0.42
86:XX:302:TYR:HD2	86:XX:345:LEU:HD21	1.83	0.42
15:1:257:LYS:O	19:5:4452:U:C4	2.72	0.42
15:1:259:LEU:CD2	15:1:259:LEU:N	2.72	0.42
19:5:1169:G:H2'	19:5:1170:G:H8	1.85	0.42
19:5:1405:C:H2'	19:5:1406:G:C8	2.51	0.42
19:5:1844:G:OP1	57:b:22:LYS:NZ	2.40	0.42
20:6:121:VAL:HG11	20:6:165:ILE:HD12	2.01	0.42
29:A:5:ILE:HD12	29:A:7:GLY:H	1.83	0.42
29:A:96:LEU:HD13	71:p:83:ILE:HG23	2.00	0.42
29:A:224:THR:HG21	29:A:243:THR:HG21	2.01	0.42
39:K:1644:C:H4'	83:UU:140:ARG:HB2	2.02	0.42
57:b:102:PRO:HA	57:b:109:ARG:HH12	1.85	0.42
77:v:233:LEU:HD12	77:v:233:LEU:HA	1.77	0.42
82:TT:8:ALA:HA	82:TT:74:VAL:HG11	2.00	0.42
86:XX:256:ILE:CD1	87:YY:37:ALA:CB	2.89	0.42
86:XX:268:LYS:HG3	86:XX:402:ARG:HD2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:JJ:6:ASP:OD1	10:JJ:6:ASP:N	2.51	0.42
13:MM:50:LYS:HD3	76:u:65:ARG:HE	1.84	0.42
15:1:259:LEU:HA	19:5:4452:U:O2	2.19	0.42
19:5:245:C:O2'	19:5:246:G:OP2	2.35	0.42
19:5:4476:C:O2	36:H:173:ARG:NH2	2.53	0.42
41:M:119:ARG:NH2	41:M:123:ILE:HD11	2.34	0.42
48:T:144:ASN:OD1	48:T:144:ASN:N	2.53	0.42
52:X:73:HIS:CD2	52:X:115:LYS:HD3	2.54	0.42
86:XX:401:MET:HG2	86:XX:409:MET:HE2	2.00	0.42
2:BB:157:HIS:HB3	2:BB:190:PRO:HG3	2.00	0.42
19:5:2404:A:H61	19:5:2787:A:H61	1.67	0.42
19:5:3723:A:H2'	19:5:3724:A:C8	2.55	0.42
19:5:4699:U:H1'	19:5:4700:A:H5''	2.01	0.42
19:5:4930:C:H5'	33:E:269:GLN:HG2	2.01	0.42
31:C:152:LEU:HD23	31:C:251:ILE:HG12	2.01	0.42
48:T:17:ARG:HD3	48:T:47:THR:HG23	2.02	0.42
61:f:50:VAL:HG22	61:f:69:VAL:HG12	2.01	0.42
81:z:57:ASP:OD2	81:z:72:ARG:NH1	2.44	0.42
85:WW:15:PHE:CE2	85:WW:22:LEU:HB2	2.55	0.42
86:XX:306:GLN:OE1	86:XX:338:VAL:HG13	2.19	0.42
87:YY:65:ILE:CG2	88:ZZ:88:HIS:CE1	3.01	0.42
16:2:64:U:H2'	16:2:65:C:H6	1.85	0.42
19:5:1308:C:H2'	19:5:1309:C:C6	2.55	0.42
19:5:1372:A:OP1	42:N:202:ARG:NH2	2.46	0.42
19:5:2362:U:H2'	19:5:2363:A:H8	1.84	0.42
22:8:102:G:OP2	22:8:104:A:O2'	2.35	0.42
24:NN:79:LEU:HA	24:NN:82:ALA:HB3	2.02	0.42
30:B:55:HIS:ND1	30:B:369:ASP:OD2	2.46	0.42
32:D:215:ASP:N	32:D:215:ASP:OD1	2.52	0.42
35:G:212:HIS:ND1	35:G:238:LYS:HA	2.34	0.42
39:K:51:U:H2'	39:K:52:G:C8	2.54	0.42
39:K:928:G:H1	39:K:1013:U:H3	1.67	0.42
39:K:1240:A:N6	85:WW:122:THR:O	2.53	0.42
39:K:1734:G:O2'	39:K:1800:A:N6	2.53	0.42
41:M:27:ILE:HD11	41:M:55:MET:HE1	2.01	0.42
43:O:80:PHE:HA	43:O:83:THR:HG22	2.01	0.42
43:O:168:TYR:CE2	43:O:172:LYS:HD2	2.55	0.42
53:Y:34:LEU:HD23	53:Y:38:LEU:HB3	2.02	0.42
81:z:53:SER:OG	81:z:110:ASN:O	2.33	0.42
86:XX:198:PRO:CG	87:YY:55:LYS:HZ2	2.32	0.42
86:XX:292:ILE:HD11	86:XX:449:LEU:HD21	1.97	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
86:XX:372:CYS:HG	86:XX:425:GLY:C	2.22	0.42
6:FF:48:GLY:HA3	80:y:145:ARG:HB2	2.00	0.42
7:GG:39:LEU:HD22	7:GG:101:ILE:HG22	2.02	0.42
15:l:248:GLN:C	15:l:249:TRP:O	2.62	0.42
19:5:1974:U:P	75:t:76:SER:HG	2.42	0.42
19:5:4458:C:OP1	30:B:11:HIS:NE2	2.52	0.42
20:6:88:ARG:NH2	39:K:1398:G:O2'	2.53	0.42
35:G:220:VAL:HG13	35:G:223:LEU:HD13	2.01	0.42
37:I:91:LEU:HD12	37:I:135:ILE:HG23	2.02	0.42
38:J:111:GLU:HG3	38:J:113:ILE:HG22	2.02	0.42
39:K:528:A:H2'	39:K:529:A:C8	2.55	0.42
39:K:1842:C:OP2	69:n:2:ARG:HD3	2.19	0.42
44:P:32:THR:HG21	44:P:87:SER:HB3	2.02	0.42
47:S:11:LYS:HD2	47:S:29:ARG:HD2	2.01	0.42
50:V:42:VAL:HB	50:V:45:ILE:HD12	2.01	0.42
50:V:106:VAL:HG21	50:V:132:ILE:HD11	2.00	0.42
53:Y:2:LYS:NZ	53:Y:4:ASN:O	2.45	0.42
55:SS:85:LEU:HB3	55:SS:89:ILE:HD11	2.02	0.42
76:u:49:VAL:HG21	76:u:62:LEU:HD22	2.01	0.42
85:WW:38:SER:OG	85:WW:39:ALA:N	2.53	0.42
86:XX:43:LEU:HD21	87:YY:50:ILE:HG12	2.01	0.42
86:XX:256:ILE:HG21	87:YY:36:ILE:HG13	2.01	0.42
86:XX:435:ALA:CB	86:XX:444:GLY:HA2	2.45	0.42
19:5:707:C:O2'	19:5:4943:A:N1	2.46	0.42
24:NN:13:MET:SD	24:NN:22:GLN:NE2	2.92	0.42
29:A:27:ALA:O	29:A:128:ARG:NH2	2.53	0.42
33:E:64:MET:HG3	33:E:68:LYS:HE3	2.01	0.42
39:K:793:G:H2'	39:K:794:A:H8	1.84	0.42
50:V:48:ARG:HB3	50:V:51:ARG:HD2	2.01	0.42
56:a:131:ARG:NH1	56:a:135:GLU:OE2	2.53	0.42
86:XX:34:TRP:CH2	88:ZZ:71:VAL:CG2	3.03	0.42
3:CC:121:LEU:HD21	3:CC:158:ILE:HD13	2.00	0.42
10:JJ:51:GLN:HA	10:JJ:66:PRO:HB3	2.01	0.42
16:2:48:C:O2'	16:2:59:A:C1'	2.68	0.42
16:2:76:A:OP1	16:2:76:A:H4'	2.20	0.42
19:5:2691:U:O2'	66:k:4:LYS:NZ	2.39	0.42
20:6:120:ILE:HB	20:6:132:TRP:HB2	2.02	0.42
22:8:52:A:N6	67:l:27:ILE:HG12	2.34	0.42
31:C:266:THR:HG23	31:C:269:LYS:H	1.85	0.42
39:K:65:C:C6	81:z:174:PRO:HB3	2.55	0.42
39:K:1143:A:H5'	77:v:190:SER:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:K:1344:A:N6	39:K:1386:A:H5'	2.35	0.42
39:K:1360:U:O2'	39:K:1379:A:OP2	2.31	0.42
40:L:9:ILE:HG12	56:a:52:TYR:CE1	2.54	0.42
44:P:88:ALA:O	44:P:92:LEU:HB2	2.20	0.42
47:S:1:MET:HB2	47:S:43:ARG:HH11	1.85	0.42
49:U:65:ARG:HG3	49:U:70:ILE:HG13	2.02	0.42
50:V:35:LYS:HB2	50:V:67:LYS:HG3	2.01	0.42
51:W:96:GLN:HE21	51:W:100:VAL:HG12	1.84	0.42
76:u:100:PHE:HB3	76:u:181:LEU:HD11	2.00	0.42
81:z:7:PHE:HB2	81:z:124:LEU:HD23	2.01	0.42
86:XX:256:ILE:HD13	87:YY:37:ALA:CA	2.50	0.42
86:XX:369:LEU:O	86:XX:426:LEU:CD1	2.64	0.42
87:YY:30:ARG:HA	87:YY:33:PHE:HB3	2.02	0.42
88:ZZ:82:ALA:HA	88:ZZ:85:PHE:HB3	2.01	0.42
15:1:252:HIS:CD2	15:1:252:HIS:H	2.38	0.41
19:5:370:U:N3	19:5:1532:G:O2'	2.48	0.41
19:5:3915:U:C3'	19:5:3915:U:C6	3.03	0.41
20:6:20:GLN:HG2	20:6:69:VAL:H	1.85	0.41
20:6:150:TRP:HB2	20:6:170:TRP:CD1	2.55	0.41
33:E:180:GLY:HA2	33:E:181:PRO:HD3	1.92	0.41
39:K:223:C:H2'	39:K:224:A:H8	1.85	0.41
39:K:399:C:H5	39:K:680:G:H5''	1.85	0.41
50:V:24:ALA:HB3	50:V:39:ILE:HD12	2.02	0.41
78:w:21:LEU:HD23	78:w:37:VAL:HG21	2.02	0.41
2:BB:144:ILE:HB	82:TT:52:ILE:HG12	2.01	0.41
19:5:282:C:O2	64:i:82:ARG:NH1	2.44	0.41
19:5:1333:A:H2'	19:5:1334:A:C8	2.55	0.41
19:5:1750:G:N2	37:I:193:ASP:OD2	2.53	0.41
19:5:1824:G:H2'	19:5:1825:A:C8	2.55	0.41
19:5:2072:C:O2'	34:F:212:LEU:O	2.32	0.41
19:5:3915:U:C6	19:5:3915:U:H3'	2.55	0.41
20:6:191:HIS:NE2	20:6:215:GLN:O	2.48	0.41
27:QQ:4:MET:HG2	27:QQ:5:HIS:CD2	2.54	0.41
30:B:56:ILE:HG22	30:B:74:GLU:HB2	2.01	0.41
30:B:288:GLY:HA3	30:B:330:PHE:CE1	2.55	0.41
33:E:142:LYS:O	33:E:194:GLN:NE2	2.44	0.41
39:K:65:C:H41	81:z:136:LYS:HB2	1.86	0.41
39:K:792:C:H2'	39:K:793:G:H8	1.85	0.41
39:K:941:C:H2'	39:K:942:G:H8	1.85	0.41
39:K:1259:A:H1'	39:K:1264:C:H42	1.86	0.41
39:K:1781:A:H2'	39:K:1782:G:C8	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:L:138:ASP:OD1	63:h:117:ARG:NH2	2.52	0.41
40:L:176:PHE:O	56:a:138:LYS:NZ	2.44	0.41
75:t:10:ILE:HG23	75:t:63:THR:HG23	2.02	0.41
82:TT:75:ILE:HD11	82:TT:93:LEU:HD11	2.02	0.41
3:CC:5:ARG:NH2	39:K:384:U:O4	2.52	0.41
8:HH:65:SER:OG	72:q:157:VAL:O	2.37	0.41
11:KK:82:ASP:O	72:q:85:ARG:NH2	2.54	0.41
17:3:28:C:H2'	17:3:29:A:C8	2.55	0.41
19:5:519:C:H2'	19:5:520:U:C6	2.55	0.41
19:5:1755:C:O2'	19:5:1757:U:OP2	2.37	0.41
19:5:1974:U:OP1	75:t:76:SER:OG	2.35	0.41
22:8:27:U:H4'	31:C:53:ALA:HB3	2.02	0.41
26:PP:132:ASP:OD2	39:K:1415:C:O2'	2.32	0.41
29:A:14:SER:H	29:A:17:ARG:HG3	1.85	0.41
31:C:60:HIS:HA	31:C:92:PHE:HE1	1.86	0.41
39:K:433:A:H2'	39:K:434:G:C8	2.55	0.41
39:K:1808:U:H2'	39:K:1809:A:C8	2.55	0.41
43:O:109:PRO:HA	43:O:110:PRO:HD3	1.88	0.41
44:P:33:ALA:HA	44:P:36:ILE:HG22	2.02	0.41
49:U:112:LEU:HD23	49:U:112:LEU:HA	1.90	0.41
77:v:178:HIS:ND1	77:v:221:ASP:OD2	2.52	0.41
78:w:93:THR:OG1	78:w:129:SER:OG	2.38	0.41
86:XX:84:ILE:HD12	86:XX:162:VAL:CG1	2.41	0.41
86:XX:256:ILE:CG2	87:YY:36:ILE:HG13	2.50	0.41
86:XX:256:ILE:CA	87:YY:36:ILE:HD11	2.50	0.41
86:XX:418:PRO:O	86:XX:421:ALA:HB3	2.20	0.41
2:BB:173:PHE:HD2	2:BB:187:PHE:HE2	1.68	0.41
3:CC:67:TRP:NE1	3:CC:191:GLU:OE2	2.46	0.41
5:EE:136:LYS:HB2	39:K:385:G:H3'	2.03	0.41
19:5:27:C:O2'	19:5:60:A:N3	2.51	0.41
19:5:1198:G:H2'	19:5:1199:G:C8	2.55	0.41
19:5:3598:C:H2'	19:5:3599:A:C8	2.55	0.41
27:QQ:33:VAL:HG21	27:QQ:66:VAL:HG11	2.01	0.41
30:B:48:GLY:HA3	30:B:81:THR:HG22	2.01	0.41
35:G:157:PRO:HG3	35:G:247:VAL:HG12	2.01	0.41
40:L:46:ILE:HB	40:L:49:ARG:HB2	2.02	0.41
41:M:24:LEU:HB2	41:M:43:THR:HG21	2.01	0.41
47:S:35:PRO:HD2	47:S:39:VAL:HG21	2.02	0.41
52:X:65:ALA:HB2	63:h:69:LEU:HD11	2.02	0.41
61:f:46:ARG:HH11	61:f:106:TYR:HE2	1.68	0.41
72:q:180:ARG:O	72:q:184:ARG:N	2.44	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
79:x:45:ILE:HG13	79:x:61:VAL:HG21	2.03	0.41
86:XX:127:GLN:HA	86:XX:130:VAL:HG12	2.02	0.41
86:XX:155:LEU:HD23	86:XX:155:LEU:HA	1.63	0.41
86:XX:256:ILE:CD1	87:YY:33:PHE:O	2.62	0.41
86:XX:291:ILE:HG21	86:XX:372:CYS:O	2.21	0.41
86:XX:454:ILE:HG23	87:YY:40:THR:CG2	2.34	0.41
9:II:88:LYS:HG2	85:WW:18:ARG:HG2	2.03	0.41
12:LL:49:ALA:O	12:LL:53:ILE:N	2.46	0.41
15:1:249:TRP:CZ2	19:5:3904:G:N3	2.88	0.41
16:2:2:C:H2'	16:2:3:U:H6	1.85	0.41
19:5:958:G:N3	33:E:127:LYS:HB2	2.35	0.41
19:5:963:G:O2'	19:5:964:A:H8	2.04	0.41
19:5:1481:C:O2'	19:5:1482:G:N3	2.39	0.41
19:5:2265:G:OP2	73:r:33:LYS:NZ	2.53	0.41
19:5:2900:U:H2'	19:5:2901:G:C8	2.55	0.41
19:5:4405:G:OP2	37:I:7:ARG:NH2	2.53	0.41
19:5:4601:U:H2'	19:5:4602:A:H8	1.84	0.41
21:7:17:C:OP1	38:J:156:ARG:NH2	2.48	0.41
24:NN:108:LYS:NZ	39:K:506:G:OP1	2.35	0.41
28:RR:54:SER:OG	28:RR:55:ASN:N	2.54	0.41
30:B:261:ARG:HB2	43:O:64:THR:HG21	2.03	0.41
37:I:61:SER:HA	37:I:126:VAL:HG23	2.02	0.41
43:O:85:ARG:HG2	43:O:99:LEU:HD11	2.03	0.41
44:P:18:ARG:HD3	44:P:147:GLU:HB3	2.03	0.41
45:Q:63:LEU:O	45:Q:67:ILE:HG12	2.20	0.41
56:a:4:ARG:H	56:a:4:ARG:HD3	1.85	0.41
76:u:31:TYR:N	76:u:47:THR:O	2.52	0.41
81:z:18:VAL:HG21	81:z:41:LEU:HD21	2.01	0.41
85:WW:17:TYR:O	85:WW:20:VAL:N	2.37	0.41
86:XX:449:LEU:HD23	86:XX:449:LEU:HA	1.69	0.41
4:DD:86:VAL:HG13	4:DD:104:ASP:HB3	2.01	0.41
13:MM:150:ARG:HD3	13:MM:150:ARG:H	1.84	0.41
19:5:966:A:O4'	19:5:968:C:N4	2.54	0.41
19:5:1925:G:H21	47:S:118:ARG:HH22	1.69	0.41
19:5:2404:A:H1'	65:j:12:ARG:HD2	2.02	0.41
19:5:2870:A:H2'	19:5:2871:A:C8	2.56	0.41
19:5:3860:A:H2	44:P:131:ARG:HH22	1.68	0.41
19:5:4594:U:H2'	19:5:4595:G:C8	2.55	0.41
29:A:175:ILE:H	29:A:175:ILE:HG13	1.50	0.41
34:F:93:ARG:HD2	34:F:113:LEU:HB3	2.03	0.41
39:K:527:C:H2'	39:K:528:A:H8	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:K:532:C:H2'	39:K:533:A:C8	2.55	0.41
55:SS:4:PRO:HD2	55:SS:7:ASN:HD22	1.86	0.41
59:d:88:LEU:HD12	59:d:88:LEU:HA	1.91	0.41
77:v:226:ALA:HB1	77:v:230:THR:HG21	2.02	0.41
86:XX:19:ILE:CG1	88:ZZ:70:PRO:CG	2.91	0.41
86:XX:34:TRP:CZ3	88:ZZ:71:VAL:HG13	2.56	0.41
86:XX:291:ILE:CG2	86:XX:372:CYS:CB	2.98	0.41
15:1:239:VAL:O	15:1:239:VAL:HG12	2.20	0.41
19:5:61:A:H5''	42:N:164:LEU:HD21	2.02	0.41
19:5:318:A:H2'	19:5:319:A:C8	2.54	0.41
19:5:461:G:H2'	19:5:462:G:C8	2.56	0.41
19:5:937:U:OP1	41:M:46:ARG:NH1	2.53	0.41
19:5:1942:A:OP2	19:5:2040:A:N6	2.47	0.41
22:8:70:G:N2	22:8:87:G:O2'	2.44	0.41
31:C:209:VAL:HB	31:C:229:LEU:HD13	2.03	0.41
34:F:103:LYS:HE3	34:F:134:ILE:HD11	2.02	0.41
48:T:63:ARG:HH22	57:b:30:GLU:CD	2.28	0.41
50:V:16:ILE:HB	50:V:88:TYR:HB2	2.01	0.41
77:v:178:HIS:O	77:v:220:ASP:N	2.50	0.41
86:XX:262:ARG:HG2	87:YY:26:THR:HG21	2.03	0.41
7:GG:56:MET:HG3	7:GG:86:LYS:HE3	2.03	0.41
12:LL:2:THR:N	39:K:1199:A:OP1	2.54	0.41
15:1:241:TYR:O	15:1:241:TYR:CD1	2.70	0.41
19:5:229:G:H5''	53:Y:11:ARG:HG3	2.03	0.41
19:5:2792:C:H2'	19:5:2793:G:H5''	2.02	0.41
20:6:60:ARG:NE	83:UU:97:GLN:HE22	2.15	0.41
21:7:105:C:OP2	37:I:203:ARG:NH2	2.54	0.41
31:C:78:ARG:HB3	31:C:88:GLY:HA2	2.02	0.41
33:E:73:ARG:HG2	33:E:75:TYR:HE2	1.85	0.41
33:E:193:HIS:CD2	33:E:195:LYS:H	2.39	0.41
39:K:51:U:H2'	39:K:52:G:H8	1.85	0.41
65:j:21:ARG:HH21	65:j:39:TYR:HA	1.85	0.41
70:o:66:ILE:H	70:o:66:ILE:HG13	1.77	0.41
72:q:69:GLU:HB3	77:v:270:THR:HG21	2.01	0.41
86:XX:47:GLN:C	86:XX:75:THR:CB	2.89	0.41
86:XX:409:MET:HB2	86:XX:409:MET:HE3	1.87	0.41
87:YY:64:ILE:HG22	88:ZZ:89:ILE:HG23	2.03	0.41
3:CC:10:LYS:HE3	3:CC:10:LYS:HB2	1.91	0.41
12:LL:5:ARG:HG3	39:K:1865:C:C2	2.56	0.41
15:1:251:ARG:NH1	19:5:4532:U:H1'	2.35	0.41
19:5:1397:A:OP1	56:a:130:SER:OG	2.31	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:5:2587:A:OP1	62:g:68:SER:OG	2.36	0.41
19:5:4518:A:OP2	30:B:258:HIS:HB2	2.21	0.41
19:5:4661:G:N2	19:5:5004:C:O3'	2.54	0.41
25:OO:80:ARG:HH21	39:K:1598:G:H3'	1.85	0.41
30:B:14:LEU:HB3	30:B:17:LEU:HD23	2.03	0.41
30:B:371:THR:HG21	51:W:17:HIS:NE2	2.36	0.41
35:G:229:LYS:HE3	35:G:229:LYS:HB3	1.88	0.41
36:H:80:MET:HE3	36:H:80:MET:HB2	1.63	0.41
39:K:5:U:H2'	39:K:6:G:C8	2.56	0.41
39:K:220:U:H2'	39:K:221:A:H8	1.85	0.41
39:K:798:G:C8	39:K:798:G:C5'	3.03	0.41
39:K:1232:U:H2'	39:K:1233:G:H8	1.85	0.41
39:K:1554:C:H3'	39:K:1555:U:H2'	2.03	0.41
45:Q:67:ILE:HD13	45:Q:98:LEU:HD11	2.02	0.41
46:R:105:LEU:HG	46:R:135:LYS:HG3	2.03	0.41
58:c:23:LYS:HE2	58:c:23:LYS:HB3	1.93	0.41
75:t:14:TYR:O	75:t:31:LYS:NZ	2.37	0.41
76:u:137:LEU:HG	76:u:215:VAL:HG22	2.03	0.41
79:x:87:MET:HE1	79:x:236:ILE:HD13	2.03	0.41
79:x:125:LYS:HB2	79:x:226:PHE:CD1	2.56	0.41
81:z:2:LYS:NZ	81:z:17:GLU:OE1	2.54	0.41
81:z:58:LYS:HE3	81:z:59:GLN:HE22	1.85	0.41
83:UU:19:ALA:HB2	83:UU:75:GLY:HA3	2.02	0.41
86:XX:10:LYS:HB3	86:XX:111:LEU:CB	2.48	0.41
86:XX:84:ILE:HD11	86:XX:162:VAL:CG1	2.51	0.41
86:XX:91:MET:SD	86:XX:116:GLN:NE2	2.89	0.41
86:XX:453:ILE:O	86:XX:457:TYR:HB2	2.20	0.41
86:XX:461:PHE:CD1	86:XX:461:PHE:C	2.98	0.41
5:EE:5:GLN:HG2	5:EE:11:GLN:HB2	2.03	0.41
7:GG:84:ILE:HD12	7:GG:84:ILE:HA	1.88	0.41
13:MM:94:HIS:CD2	13:MM:128:ARG:H	2.39	0.41
19:5:223:G:H4'	19:5:225:G:N7	2.36	0.41
19:5:1217:G:H2'	19:5:1218:G:H8	1.86	0.41
19:5:1919:G:N2	47:S:163:HIS:O	2.43	0.41
19:5:2492:C:H2'	19:5:2493:G:C8	2.55	0.41
22:8:154:G:H4'	35:G:242:ARG:HH12	1.86	0.41
23:9:26:ASN:ND2	39:K:1495:G:O2'	2.54	0.41
29:A:104:VAL:HG12	29:A:146:THR:HG21	2.02	0.41
56:a:12:ARG:HA	56:a:12:ARG:HD3	1.86	0.41
86:XX:121:MET:CE	86:XX:156:PHE:HD1	2.34	0.41
86:XX:441:ILE:CG1	86:XX:444:GLY:H	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:II:91:LYS:O	85:WW:16:THR:OG1	2.32	0.40
19:5:364:G:O6	65:j:52:LYS:NZ	2.44	0.40
19:5:1458:C:H5''	45:Q:69:LYS:HD2	2.03	0.40
19:5:2479:G:H2'	19:5:2480:G:H8	1.85	0.40
19:5:4099:G:N2	19:5:4109:G:H1	2.17	0.40
19:5:4271:A:OP1	19:5:4272:G:N2	2.54	0.40
19:5:4380:A:OP1	70:o:58:LYS:NZ	2.52	0.40
22:8:75:G:OP2	53:Y:74:TYR:OH	2.36	0.40
24:NN:15:ASN:HD22	24:NN:20:ARG:HD2	1.86	0.40
24:NN:37:LYS:HG3	39:K:571:U:H5''	2.02	0.40
25:OO:50:PHE:HB3	25:OO:55:TYR:HB2	2.03	0.40
37:I:159:PHE:HB2	37:I:163:GLN:HE22	1.85	0.40
38:J:56:THR:HG23	38:J:63:ARG:HA	2.04	0.40
39:K:1:U:H6	77:v:205:VAL:HG13	1.86	0.40
45:Q:178:ARG:HB2	56:a:53:PHE:O	2.21	0.40
53:Y:31:SER:HA	53:Y:48:PRO:HA	2.02	0.40
73:r:52:GLU:HB2	73:r:61:VAL:HG22	2.04	0.40
5:EE:90:ARG:HD3	5:EE:109:MET:HE3	2.03	0.40
16:2:31:G:H1	16:2:39:U:H3	1.68	0.40
19:5:108:A:N1	19:5:333:U:O2'	2.54	0.40
19:5:1849:U:H3'	40:L:5:ARG:HH12	1.86	0.40
19:5:4680:G:H2'	19:5:4681:A:C8	2.55	0.40
39:K:639:C:H2'	39:K:640:A:H8	1.85	0.40
39:K:1098:C:H2'	39:K:1099:G:C8	2.56	0.40
39:K:1226:G:N1	39:K:1639:G:OP2	2.41	0.40
39:K:1298:G:O2'	39:K:1299:A:O4'	2.39	0.40
39:K:1753:C:H2'	39:K:1754:G:H8	1.86	0.40
61:f:87:LYS:HE2	61:f:87:LYS:HB2	1.90	0.40
86:XX:184:ALA:HB2	86:XX:453:ILE:HG21	2.04	0.40
87:YY:68:GLY:HA3	88:ZZ:95:ARG:O	2.09	0.40
6:FF:44:ARG:NH2	80:y:140:ASP:OD2	2.54	0.40
15:1:256:TRP:CG	19:5:3904:G:H22	2.39	0.40
19:5:16:G:OP1	52:X:62:ARG:NH2	2.54	0.40
19:5:1802:A:O2'	19:5:1837:A:OP1	2.37	0.40
19:5:1995:G:O6	19:5:2000:G:N2	2.54	0.40
19:5:2517:A:O4'	62:g:62:LYS:HD2	2.22	0.40
19:5:2864:A:H5''	46:R:84:THR:HG22	2.03	0.40
19:5:3827:G:O2'	19:5:3829:G:OP2	2.35	0.40
19:5:4460:U:H2'	19:5:4461:C:C6	2.57	0.40
19:5:5057:C:H2'	19:5:5058:A:C8	2.56	0.40
22:8:141:C:H2'	22:8:142:U:C6	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:A:108:PRO:HD3	71:p:90:LYS:HE3	2.03	0.40
30:B:276:HIS:O	30:B:277:ARG:NH1	2.49	0.40
30:B:337:VAL:HG21	30:B:345:LEU:HD21	2.03	0.40
39:K:85:A:H2'	39:K:86:C:H6	1.85	0.40
49:U:46:ARG:HH22	49:U:89:LYS:HE2	1.86	0.40
49:U:84:LYS:HA	49:U:87:THR:HG22	2.02	0.40
60:e:85:LEU:HD11	60:e:111:ILE:HG23	2.02	0.40
79:x:99:PHE:HE1	79:x:113:ARG:HG2	1.85	0.40
86:XX:173:TYR:CZ	86:XX:175:LEU:HB2	2.57	0.40
86:XX:247:ALA:O	86:XX:440:ALA:HB3	2.13	0.40
86:XX:428:ILE:HG23	86:XX:448:LEU:CD2	2.52	0.40
13:MM:50:LYS:NZ	39:K:951:C:O2'	2.54	0.40
16:2:20:C:O2	16:2:20:C:C5'	2.69	0.40
19:5:423:G:H5'	44:P:26:PHE:HZ	1.87	0.40
19:5:2638:G:H4'	62:g:24:ARG:HD3	2.04	0.40
19:5:4305:G:N2	48:T:87:LYS:HZ2	2.19	0.40
31:C:262:ASP:HB3	31:C:273:LEU:HD13	2.04	0.40
32:D:128:ASP:O	32:D:164:LYS:NZ	2.48	0.40
40:L:106:SER:HG	40:L:109:SER:HG	1.67	0.40
58:c:31:TYR:O	58:c:35:LEU:HB2	2.22	0.40
88:ZZ:68:VAL:HA	88:ZZ:70:PRO:HD2	2.02	0.40
4:DD:10:ARG:NH2	39:K:816:A:OP2	2.54	0.40
16:2:18:G:H5''	16:2:18:G:H8	1.85	0.40
16:2:20:C:O2	16:2:20:C:C2'	2.69	0.40
19:5:3937:C:O2'	42:N:124:ASP:OD1	2.39	0.40
19:5:5002:U:H2'	19:5:5003:U:C6	2.56	0.40
20:6:46:THR:HG21	20:6:54:ILE:HD12	2.03	0.40
39:K:64:A:OP1	81:z:177:GLN:NE2	2.53	0.40
39:K:434:G:H2'	39:K:435:A:C8	2.56	0.40
39:K:1097:G:H4'	72:q:32:PHE:CG	2.56	0.40
39:K:1368:U:O2'	39:K:1370:A:N7	2.50	0.40
39:K:1650:A:H5''	83:UU:139:ALA:HB2	2.04	0.40
43:O:12:ARG:O	47:S:171:ARG:NH2	2.55	0.40
44:P:36:ILE:HG21	44:P:36:ILE:HD13	1.89	0.40
47:S:9:GLU:HG3	47:S:33:PHE:CE1	2.57	0.40
52:X:83:THR:O	52:X:87:MET:N	2.47	0.40
56:a:82:VAL:HG12	56:a:86:THR:HG21	2.04	0.40
59:d:19:GLU:OE1	59:d:92:ARG:NH1	2.55	0.40
60:e:99:ILE:HG21	60:e:108:ARG:HG2	2.03	0.40
70:o:85:ILE:HG22	70:o:86:LYS:H	1.86	0.40
77:v:125:LYS:HE2	77:v:127:PHE:HE1	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
79:x:125:LYS:HB2	79:x:226:PHE:HD1	1.87	0.40
79:x:245:ARG:HD2	79:x:245:ARG:HA	1.91	0.40
86:XX:173:TYR:CE1	86:XX:175:LEU:HD13	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AA	53/55 (96%)	51 (96%)	2 (4%)	0	100	100
2	BB	181/189 (96%)	174 (96%)	7 (4%)	0	100	100
3	CC	204/206 (99%)	194 (95%)	10 (5%)	0	100	100
4	DD	183/185 (99%)	179 (98%)	4 (2%)	0	100	100
5	EE	139/151 (92%)	132 (95%)	7 (5%)	0	100	100
6	FF	60/62 (97%)	57 (95%)	3 (5%)	0	100	100
7	GG	98/100 (98%)	95 (97%)	3 (3%)	0	100	100
8	HH	81/83 (98%)	76 (94%)	5 (6%)	0	100	100
9	II	142/144 (99%)	135 (95%)	7 (5%)	0	100	100
10	JJ	81/83 (98%)	77 (95%)	4 (5%)	0	100	100
11	KK	130/132 (98%)	123 (95%)	7 (5%)	0	100	100
12	LL	99/101 (98%)	91 (92%)	8 (8%)	0	100	100
13	MM	134/136 (98%)	126 (94%)	8 (6%)	0	100	100
14	0	66/68 (97%)	61 (92%)	5 (8%)	0	100	100
15	1	22/24 (92%)	13 (59%)	7 (32%)	2 (9%)	0	9
20	6	311/313 (99%)	283 (91%)	28 (9%)	0	100	100
23	9	53/55 (96%)	51 (96%)	2 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	NN	122/124 (98%)	119 (98%)	3 (2%)	0	100	100
25	OO	73/75 (97%)	70 (96%)	3 (4%)	0	100	100
26	PP	139/141 (99%)	130 (94%)	9 (6%)	0	100	100
27	QQ	147/149 (99%)	145 (99%)	2 (1%)	0	100	100
28	RR	115/117 (98%)	104 (90%)	11 (10%)	0	100	100
29	A	246/248 (99%)	231 (94%)	15 (6%)	0	100	100
30	B	392/394 (100%)	368 (94%)	24 (6%)	0	100	100
31	C	360/362 (99%)	341 (95%)	19 (5%)	0	100	100
32	D	291/293 (99%)	281 (97%)	10 (3%)	0	100	100
33	E	208/251 (83%)	195 (94%)	13 (6%)	0	100	100
34	F	223/225 (99%)	214 (96%)	9 (4%)	0	100	100
35	G	229/240 (95%)	222 (97%)	7 (3%)	0	100	100
36	H	188/190 (99%)	178 (95%)	10 (5%)	0	100	100
37	I	201/213 (94%)	191 (95%)	10 (5%)	0	100	100
38	J	168/170 (99%)	162 (96%)	6 (4%)	0	100	100
40	L	208/210 (99%)	198 (95%)	7 (3%)	3 (1%)	9	38
41	M	136/138 (99%)	130 (96%)	6 (4%)	0	100	100
42	N	201/203 (99%)	189 (94%)	12 (6%)	0	100	100
43	O	197/199 (99%)	191 (97%)	6 (3%)	0	100	100
44	P	151/153 (99%)	145 (96%)	6 (4%)	0	100	100
45	Q	185/187 (99%)	177 (96%)	8 (4%)	0	100	100
46	R	178/180 (99%)	175 (98%)	3 (2%)	0	100	100
47	S	174/176 (99%)	165 (95%)	9 (5%)	0	100	100
48	T	157/159 (99%)	147 (94%)	10 (6%)	0	100	100
49	U	97/99 (98%)	91 (94%)	6 (6%)	0	100	100
50	V	129/131 (98%)	123 (95%)	6 (5%)	0	100	100
51	W	102/121 (84%)	98 (96%)	4 (4%)	0	100	100
52	X	116/118 (98%)	113 (97%)	3 (3%)	0	100	100
53	Y	132/134 (98%)	129 (98%)	3 (2%)	0	100	100
54	Z	133/135 (98%)	128 (96%)	4 (3%)	1 (1%)	16	50
55	SS	94/96 (98%)	88 (94%)	6 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
56	a	145/147 (99%)	139 (96%)	6 (4%)	0	100	100
57	b	100/116 (86%)	96 (96%)	4 (4%)	0	100	100
58	c	96/98 (98%)	93 (97%)	3 (3%)	0	100	100
59	d	105/107 (98%)	97 (92%)	8 (8%)	0	100	100
60	e	126/128 (98%)	122 (97%)	4 (3%)	0	100	100
61	f	107/109 (98%)	102 (95%)	5 (5%)	0	100	100
62	g	112/114 (98%)	110 (98%)	2 (2%)	0	100	100
63	h	120/122 (98%)	117 (98%)	3 (2%)	0	100	100
64	i	100/102 (98%)	97 (97%)	3 (3%)	0	100	100
65	j	84/86 (98%)	82 (98%)	2 (2%)	0	100	100
66	k	67/69 (97%)	66 (98%)	1 (2%)	0	100	100
67	l	48/50 (96%)	45 (94%)	3 (6%)	0	100	100
68	m	50/52 (96%)	49 (98%)	1 (2%)	0	100	100
69	n	23/25 (92%)	23 (100%)	0	0	100	100
70	o	102/104 (98%)	97 (95%)	5 (5%)	0	100	100
71	p	89/91 (98%)	86 (97%)	3 (3%)	0	100	100
72	q	215/217 (99%)	202 (94%)	13 (6%)	0	100	100
73	r	122/124 (98%)	113 (93%)	9 (7%)	0	100	100
74	s	194/196 (99%)	181 (93%)	13 (7%)	0	100	100
75	t	151/153 (99%)	135 (89%)	16 (11%)	0	100	100
76	u	211/213 (99%)	202 (96%)	9 (4%)	0	100	100
77	v	219/221 (99%)	213 (97%)	6 (3%)	0	100	100
78	w	226/228 (99%)	218 (96%)	8 (4%)	0	100	100
79	x	260/262 (99%)	249 (96%)	11 (4%)	0	100	100
80	y	181/191 (95%)	169 (93%)	12 (7%)	0	100	100
81	z	235/237 (99%)	228 (97%)	7 (3%)	0	100	100
82	TT	127/129 (98%)	119 (94%)	8 (6%)	0	100	100
83	UU	140/142 (99%)	133 (95%)	7 (5%)	0	100	100
84	VV	139/141 (99%)	132 (95%)	5 (4%)	2 (1%)	9	38
85	WW	118/120 (98%)	111 (94%)	6 (5%)	1 (1%)	16	50
86	XX	412/461 (89%)	363 (88%)	45 (11%)	4 (1%)	12	45

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
87	YY	60/62 (97%)	50 (83%)	8 (13%)	2 (3%)	3	24
88	ZZ	27/29 (93%)	25 (93%)	1 (4%)	1 (4%)	2	22
All	All	12040/12364 (97%)	11420 (95%)	604 (5%)	16 (0%)	49	80

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	1	249	TRP
86	XX	107	LYS
86	XX	108	ASP
86	XX	445	THR
40	L	64	VAL
84	VV	62	PRO
15	1	258	PRO
40	L	5	ARG
40	L	63	THR
86	XX	286	THR
87	YY	31	LYS
84	VV	86	PRO
85	WW	18	ARG
54	Z	90	PRO
87	YY	28	PRO
88	ZZ	71	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AA	46/46 (100%)	46 (100%)	0	100	100
2	BB	165/169 (98%)	165 (100%)	0	100	100
3	CC	178/178 (100%)	176 (99%)	2 (1%)	65	74
4	DD	161/161 (100%)	161 (100%)	0	100	100
5	EE	130/136 (96%)	130 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	FF	55/55 (100%)	55 (100%)	0	100	100
7	GG	92/92 (100%)	92 (100%)	0	100	100
8	HH	67/67 (100%)	66 (98%)	1 (2%)	57	70
9	II	125/125 (100%)	124 (99%)	1 (1%)	73	77
10	JJ	75/75 (100%)	75 (100%)	0	100	100
11	KK	119/119 (100%)	119 (100%)	0	100	100
12	LL	88/88 (100%)	88 (100%)	0	100	100
13	MM	106/106 (100%)	106 (100%)	0	100	100
14	0	61/61 (100%)	61 (100%)	0	100	100
15	1	22/22 (100%)	14 (64%)	8 (36%)	0	1
20	6	272/272 (100%)	272 (100%)	0	100	100
23	9	48/48 (100%)	48 (100%)	0	100	100
24	NN	107/107 (100%)	106 (99%)	1 (1%)	70	75
25	OO	66/66 (100%)	66 (100%)	0	100	100
26	PP	111/111 (100%)	110 (99%)	1 (1%)	70	75
27	QQ	130/130 (100%)	129 (99%)	1 (1%)	73	77
28	RR	99/99 (100%)	99 (100%)	0	100	100
29	A	190/190 (100%)	185 (97%)	5 (3%)	40	60
30	B	342/342 (100%)	336 (98%)	6 (2%)	51	67
31	C	302/302 (100%)	296 (98%)	6 (2%)	48	65
32	D	247/247 (100%)	246 (100%)	1 (0%)	84	83
33	E	190/223 (85%)	189 (100%)	1 (0%)	81	82
34	F	196/196 (100%)	193 (98%)	3 (2%)	57	70
35	G	200/205 (98%)	199 (100%)	1 (0%)	81	82
36	H	169/169 (100%)	169 (100%)	0	100	100
37	I	175/180 (97%)	175 (100%)	0	100	100
38	J	143/143 (100%)	140 (98%)	3 (2%)	47	65
40	L	175/175 (100%)	172 (98%)	3 (2%)	53	68
41	M	117/117 (100%)	115 (98%)	2 (2%)	53	68
42	N	171/171 (100%)	168 (98%)	3 (2%)	51	67
43	O	171/171 (100%)	171 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
44	P	134/134 (100%)	133 (99%)	1 (1%)	76	78
45	Q	164/164 (100%)	162 (99%)	2 (1%)	63	72
46	R	159/159 (100%)	158 (99%)	1 (1%)	78	80
47	S	157/157 (100%)	153 (98%)	4 (2%)	42	62
48	T	139/139 (100%)	137 (99%)	2 (1%)	59	71
49	U	89/89 (100%)	89 (100%)	0	100	100
50	V	101/101 (100%)	99 (98%)	2 (2%)	48	65
51	W	86/100 (86%)	86 (100%)	0	100	100
52	X	106/106 (100%)	105 (99%)	1 (1%)	70	75
53	Y	124/124 (100%)	121 (98%)	3 (2%)	43	63
54	Z	117/117 (100%)	116 (99%)	1 (1%)	70	75
55	SS	87/87 (100%)	86 (99%)	1 (1%)	65	74
56	a	119/119 (100%)	118 (99%)	1 (1%)	73	77
57	b	84/95 (88%)	83 (99%)	1 (1%)	63	72
58	c	84/84 (100%)	84 (100%)	0	100	100
59	d	98/98 (100%)	98 (100%)	0	100	100
60	e	114/114 (100%)	114 (100%)	0	100	100
61	f	88/88 (100%)	86 (98%)	2 (2%)	44	63
62	g	98/98 (100%)	94 (96%)	4 (4%)	27	51
63	h	109/109 (100%)	109 (100%)	0	100	100
64	i	86/86 (100%)	85 (99%)	1 (1%)	63	72
65	j	73/73 (100%)	73 (100%)	0	100	100
66	k	64/64 (100%)	63 (98%)	1 (2%)	55	69
67	l	47/47 (100%)	47 (100%)	0	100	100
68	m	48/48 (100%)	47 (98%)	1 (2%)	47	65
69	n	24/24 (100%)	23 (96%)	1 (4%)	26	50
70	o	92/92 (100%)	92 (100%)	0	100	100
71	p	74/74 (100%)	71 (96%)	3 (4%)	27	51
72	q	180/181 (99%)	179 (99%)	1 (1%)	78	80
73	r	108/108 (100%)	106 (98%)	2 (2%)	50	66
74	s	164/164 (100%)	164 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
75	t	126/126 (100%)	125 (99%)	1 (1%)	73	77
76	u	194/194 (100%)	192 (99%)	2 (1%)	68	75
77	v	187/187 (100%)	185 (99%)	2 (1%)	65	74
78	w	190/190 (100%)	190 (100%)	0	100	100
79	x	224/224 (100%)	224 (100%)	0	100	100
80	y	158/161 (98%)	157 (99%)	1 (1%)	78	80
81	z	207/207 (100%)	206 (100%)	1 (0%)	81	82
82	TT	112/112 (100%)	111 (99%)	1 (1%)	70	75
83	UU	117/117 (100%)	117 (100%)	0	100	100
84	VV	113/113 (100%)	112 (99%)	1 (1%)	70	75
85	WW	109/109 (100%)	109 (100%)	0	100	100
86	XX	360/387 (93%)	344 (96%)	16 (4%)	25	49
87	YY	53/53 (100%)	45 (85%)	8 (15%)	3	16
88	ZZ	26/26 (100%)	20 (77%)	6 (23%)	1	5
All	All	10504/10613 (99%)	10380 (99%)	124 (1%)	61	72

All (124) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	CC	36	THR
3	CC	121	LEU
8	HH	11	LEU
9	II	8	LYS
15	1	237	ASP
15	1	239	VAL
15	1	241	TYR
15	1	246	LEU
15	1	251	ARG
15	1	253	GLN
15	1	257	LYS
15	1	259	LEU
24	NN	17	LEU
26	PP	124	THR
27	QQ	60	VAL
29	A	82	ILE
29	A	101	VAL
29	A	200	ARG

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Mol	Chain	Res	Type
29	A	207	VAL
29	A	243	THR
30	B	56	ILE
30	B	66	LYS
30	B	162	VAL
30	B	262	VAL
30	B	314	ILE
30	B	363	ILE
31	C	150	LEU
31	C	154	VAL
31	C	223	ASN
31	C	232	VAL
31	C	321	ASN
31	C	322	LEU
32	D	226	TYR
33	E	52	LEU
34	F	88	LEU
34	F	100	VAL
34	F	151	GLU
35	G	220	VAL
38	J	33	LEU
38	J	49	VAL
38	J	83	LEU
40	L	59	VAL
40	L	63	THR
40	L	154	VAL
41	M	25	VAL
41	M	38	VAL
42	N	64	ILE
42	N	89	VAL
42	N	151	ILE
44	P	128	ARG
45	Q	5	ILE
45	Q	172	ARG
46	R	50	ILE
47	S	9	GLU
47	S	13	VAL
47	S	67	VAL
47	S	90	THR
48	T	96	ILE
48	T	136	ARG
50	V	18	LEU

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Mol	Chain	Res	Type
50	V	61	VAL
52	X	53	ARG
53	Y	55	VAL
53	Y	79	VAL
53	Y	104	VAL
54	Z	68	ILE
55	SS	35	LEU
56	a	122	VAL
57	b	72	ILE
61	f	33	VAL
61	f	88	PHE
62	g	5	LEU
62	g	15	THR
62	g	18	ASN
62	g	43	LYS
64	i	17	VAL
66	k	69	LEU
68	m	59	LEU
69	n	13	LEU
71	p	29	ILE
71	p	52	VAL
71	p	54	ILE
72	q	173	LEU
73	r	12	ASN
73	r	78	VAL
75	t	37	LEU
76	u	63	LYS
76	u	207	LEU
77	v	137	VAL
77	v	167	ARG
80	y	173	LEU
81	z	63	MET
82	TT	104	LEU
84	VV	7	LEU
86	XX	45	CYS
86	XX	64	TRP
86	XX	65	MET
86	XX	66	ARG
86	XX	68	ILE
86	XX	187	ILE
86	XX	192	VAL
86	XX	249	ILE

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Mol	Chain	Res	Type
86	XX	251	VAL
86	XX	355	LEU
86	XX	406	GLU
86	XX	436	ASP
86	XX	438	LEU
86	XX	441	ILE
86	XX	458	PHE
86	XX	462	VAL
87	YY	26	THR
87	YY	27	LYS
87	YY	29	ASP
87	YY	30	ARG
87	YY	31	LYS
87	YY	32	GLU
87	YY	40	THR
87	YY	59	ILE
88	ZZ	73	VAL
88	ZZ	76	MET
88	ZZ	78	LEU
88	ZZ	79	LEU
88	ZZ	81	ILE
88	ZZ	87	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (179) such sidechains are listed below:

Mol	Chain	Res	Type
1	AA	88	GLN
1	AA	95	GLN
1	AA	117	ASN
2	BB	97	GLN
2	BB	126	HIS
2	BB	168	HIS
3	CC	7	ASN
3	CC	84	ASN
3	CC	87	ASN
3	CC	99	ASN
4	DD	124	HIS
4	DD	154	GLN
5	EE	19	ASN
5	EE	94	HIS
5	EE	112	HIS
5	EE	121	GLN

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Mol	Chain	Res	Type
6	FF	26	GLN
6	FF	29	GLN
7	GG	47	ASN
7	GG	92	HIS
8	HH	47	ASN
11	KK	31	ASN
11	KK	62	GLN
11	KK	74	GLN
13	MM	94	HIS
15	1	252	HIS
15	1	253	GLN
20	6	133	ASN
20	6	159	ASN
20	6	178	ASN
20	6	196	ASN
23	9	26	ASN
24	NN	15	ASN
24	NN	22	GLN
24	NN	112	ASN
27	QQ	62	GLN
27	QQ	90	HIS
27	QQ	105	ASN
28	RR	19	GLN
28	RR	48	HIS
28	RR	72	HIS
28	RR	82	ASN
29	A	139	HIS
29	A	194	ASN
29	A	205	ASN
29	A	216	HIS
30	B	121	ASN
30	B	179	HIS
30	B	203	GLN
30	B	236	HIS
31	C	38	ASN
31	C	50	GLN
31	C	187	GLN
31	C	223	ASN
31	C	321	ASN
31	C	329	ASN
32	D	111	ASN
32	D	138	GLN

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Mol	Chain	Res	Type
32	D	175	HIS
32	D	222	GLN
33	E	45	HIS
33	E	185	ASN
33	E	193	HIS
34	F	38	GLN
34	F	79	ASN
34	F	205	ASN
35	G	117	GLN
35	G	134	ASN
35	G	259	GLN
35	G	293	ASN
36	H	8	GLN
36	H	15	ASN
36	H	39	ASN
36	H	78	GLN
36	H	98	HIS
36	H	102	ASN
37	I	73	ASN
37	I	95	HIS
37	I	100	ASN
38	J	98	ASN
40	L	67	HIS
40	L	113	ASN
41	M	66	HIS
41	M	83	ASN
42	N	8	GLN
42	N	109	HIS
42	N	196	ASN
43	O	50	ASN
44	P	120	ASN
44	P	133	HIS
44	P	137	ASN
45	Q	125	GLN
46	R	36	ASN
46	R	75	HIS
46	R	130	ASN
46	R	141	HIS
46	R	178	GLN
48	T	22	HIS
48	T	54	HIS
48	T	98	HIS

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Mol	Chain	Res	Type
48	T	139	HIS
50	V	77	HIS
51	W	30	GLN
51	W	50	ASN
51	W	96	GLN
51	W	120	GLN
52	X	93	ASN
52	X	105	ASN
52	X	107	HIS
52	X	111	GLN
52	X	151	ASN
53	Y	14	ASN
55	SS	7	ASN
55	SS	28	HIS
55	SS	84	HIS
57	b	6	ASN
57	b	12	GLN
57	b	50	ASN
59	d	18	ASN
59	d	30	HIS
59	d	79	ASN
62	g	14	ASN
62	g	18	ASN
62	g	114	GLN
64	i	15	HIS
65	j	76	HIS
68	m	61	GLN
68	m	78	HIS
68	m	94	ASN
70	o	45	GLN
71	p	33	GLN
72	q	81	ASN
73	r	12	ASN
73	r	45	HIS
73	r	103	HIS
74	s	126	GLN
75	t	65	GLN
75	t	115	GLN
76	u	147	ASN
76	u	157	GLN
76	u	158	HIS
77	v	136	HIS

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Mol	Chain	Res	Type
77	v	272	HIS
78	w	22	ASN
79	x	112	HIS
79	x	138	HIS
79	x	142	HIS
79	x	188	ASN
79	x	232	ASN
80	y	31	ASN
80	y	79	HIS
81	z	65	GLN
81	z	81	HIS
81	z	177	GLN
81	z	186	GLN
81	z	202	ASN
82	TT	15	ASN
82	TT	56	HIS
82	TT	113	HIS
83	UU	11	GLN
83	UU	77	HIS
83	UU	80	GLN
83	UU	97	GLN
84	VV	16	HIS
84	VV	31	HIS
84	VV	46	HIS
85	WW	41	GLN
85	WW	104	GLN
86	XX	72	ASN
86	XX	116	GLN
86	XX	218	HIS
86	XX	241	ASN
86	XX	244	ASN
86	XX	300	ASN
86	XX	343	HIS
86	XX	393	GLN
86	XX	414	ASN
87	YY	58	HIS
87	YY	63	ASN

5.3.3 RNA ⓘ

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
16	2	73/75 (97%)	26 (35%)	2 (2%)
17	3	72/75 (96%)	16 (22%)	0
18	4	5/6 (83%)	1 (20%)	0
19	5	3519/3544 (99%)	843 (23%)	73 (2%)
21	7	119/120 (99%)	14 (11%)	0
22	8	149/151 (98%)	26 (17%)	1 (0%)
39	K	1686/1698 (99%)	397 (23%)	25 (1%)
All	All	5623/5669 (99%)	1323 (23%)	101 (1%)

All (1323) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
16	2	2	C
16	2	5	C
16	2	8	U
16	2	9	A
16	2	16	C
16	2	19	G
16	2	20	C
16	2	21	A
16	2	22	G
16	2	25	C
16	2	35	A
16	2	42	A
16	2	46	G
16	2	47	U
16	2	48	C
16	2	51	U
16	2	52	G
16	2	53	G
16	2	54	U
16	2	58	A
16	2	59	A
16	2	60	A
16	2	61	C
16	2	62	C
16	2	64	U
16	2	76	A
17	3	7	A
17	3	13	C
17	3	16	C

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Mol	Chain	Res	Type
17	3	19	G
17	3	21	A
17	3	34	U
17	3	35	A
17	3	42	G
17	3	48	C
17	3	49	C
17	3	58	A
17	3	63	C
17	3	69	G
17	3	70	G
17	3	74	C
17	3	76	A
18	4	46	A
19	5	5	A
19	5	8	U
19	5	12	A
19	5	13	U
19	5	17	A
19	5	25	A
19	5	30	C
19	5	34	A
19	5	39	A
19	5	42	A
19	5	44	A
19	5	48	G
19	5	49	U
19	5	56	A
19	5	57	G
19	5	58	G
19	5	59	A
19	5	64	A
19	5	65	A
19	5	72	C
19	5	73	A
19	5	74	G
19	5	77	U
19	5	84	A
19	5	85	G
19	5	91	G
19	5	93	G
19	5	98	A

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Mol	Chain	Res	Type
19	5	104	G
19	5	108	A
19	5	109	G
19	5	112	C
19	5	116	G
19	5	118	C
19	5	119	G
19	5	126	C
19	5	134	G
19	5	135	G
19	5	136	C
19	5	142	G
19	5	143	C
19	5	146	G
19	5	157	U
19	5	159	C
19	5	170	C
19	5	171	U
19	5	172	C
19	5	173	C
19	5	177	G
19	5	179	G
19	5	182	G
19	5	200	U
19	5	201	C
19	5	209	U
19	5	216	C
19	5	218	A
19	5	220	C
19	5	224	U
19	5	226	G
19	5	233	U
19	5	234	G
19	5	245	C
19	5	246	G
19	5	255	C
19	5	256	G
19	5	262	G
19	5	265	C
19	5	266	C
19	5	276	C
19	5	277	G

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Mol	Chain	Res	Type
19	5	278	G
19	5	280	G
19	5	292	G
19	5	297	U
19	5	306	A
19	5	309	C
19	5	310	G
19	5	315	G
19	5	316	U
19	5	322	C
19	5	334	A
19	5	340	C
19	5	345	C
19	5	350	C
19	5	363	A
19	5	387	G
19	5	407	A
19	5	408	A
19	5	409	G
19	5	410	A
19	5	412	G
19	5	413	G
19	5	431	G
19	5	432	U
19	5	445	U
19	5	449	C
19	5	450	G
19	5	452	A
19	5	453	G
19	5	454	U
19	5	455	C
19	5	456	C
19	5	463	A
19	5	466	A
19	5	467	U
19	5	468	U
19	5	481	G
19	5	481(A)	C
19	5	482	G
19	5	483	G
19	5	485	C
19	5	486	C

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Mol	Chain	Res	Type
19	5	492	U
19	5	493	G
19	5	495	C
19	5	497	G
19	5	498	C
19	5	499	G
19	5	505	G
19	5	506	C
19	5	510	U
19	5	522	C
19	5	647	G
19	5	658	C
19	5	666	G
19	5	667	A
19	5	668	C
19	5	669	C
19	5	683	C
19	5	684	G
19	5	685	C
19	5	686	A
19	5	687	U
19	5	696	C
19	5	697	G
19	5	704	C
19	5	705	G
19	5	719	C
19	5	722	G
19	5	729	G
19	5	730	G
19	5	731	G
19	5	738	C
19	5	738(A)	C
19	5	742	G
19	5	747	A
19	5	749	G
19	5	751	G
19	5	752	G
19	5	758	G
19	5	908	G
19	5	913	U
19	5	914	U
19	5	915	A

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Mol	Chain	Res	Type
19	5	917	A
19	5	918	G
19	5	923	C
19	5	925	C
19	5	926	G
19	5	928	C
19	5	929	A
19	5	931	C
19	5	932	A
19	5	933	G
19	5	934	C
19	5	935	A
19	5	935(A)	G
19	5	936	C
19	5	939	G
19	5	941	C
19	5	943	A
19	5	945	U
19	5	958	G
19	5	959	G
19	5	960	A
19	5	961	G
19	5	962	C
19	5	964	A
19	5	965	G
19	5	966	A
19	5	967	C
19	5	969	C
19	5	971(A)	G
19	5	972	C
19	5	979	C
19	5	983	C
19	5	1070	G
19	5	1072	C
19	5	1073	G
19	5	1075	G
19	5	1076	C
19	5	1078	A
19	5	1079	C
19	5	1081	C
19	5	1175	A
19	5	1179	U

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Mol	Chain	Res	Type
19	5	1180	C
19	5	1187	G
19	5	1191	C
19	5	1193	C
19	5	1204	C
19	5	1210	C
19	5	1211	G
19	5	1212	G
19	5	1215	C
19	5	1234	G
19	5	1235	G
19	5	1236	C
19	5	1237	C
19	5	1238	A
19	5	1239	C
19	5	1272	C
19	5	1273	G
19	5	1275	G
19	5	1276	C
19	5	1277	G
19	5	1284	G
19	5	1287	G
19	5	1292	C
19	5	1293	G
19	5	1295	U
19	5	1296	G
19	5	1301	C
19	5	1303	A
19	5	1304	C
19	5	1326	A
19	5	1330	A
19	5	1354	A
19	5	1358	G
19	5	1359	G
19	5	1370	G
19	5	1371	A
19	5	1377	G
19	5	1378	C
19	5	1387	A
19	5	1394	G
19	5	1397	A
19	5	1398	A

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Mol	Chain	Res	Type
19	5	1400	G
19	5	1414	C
19	5	1415	G
19	5	1419	G
19	5	1420	A
19	5	1421	G
19	5	1426	G
19	5	1436	C
19	5	1437	C
19	5	1438	U
19	5	1441	C
19	5	1445	U
19	5	1446	C
19	5	1448	G
19	5	1456	C
19	5	1457	G
19	5	1458	C
19	5	1475	G
19	5	1478	C
19	5	1482	G
19	5	1483	C
19	5	1484	G
19	5	1494	U
19	5	1497	A
19	5	1498	G
19	5	1502	G
19	5	1515	A
19	5	1518	A
19	5	1523	A
19	5	1525	A
19	5	1534	A
19	5	1546	C
19	5	1547	A
19	5	1563	A
19	5	1564	A
19	5	1566	C
19	5	1574	G
19	5	1578	U
19	5	1586	G
19	5	1591	U
19	5	1596	U
19	5	1597	G

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Mol	Chain	Res	Type
19	5	1602	U
19	5	1612	G
19	5	1613	A
19	5	1624	G
19	5	1625	G
19	5	1631	A
19	5	1633	G
19	5	1634	A
19	5	1638	A
19	5	1640	C
19	5	1641	G
19	5	1642	A
19	5	1654	G
19	5	1661	C
19	5	1676	C
19	5	1677	U
19	5	1678	C
19	5	1680	G
19	5	1691	G
19	5	1724	G
19	5	1731	C
19	5	1734	G
19	5	1741	G
19	5	1742	A
19	5	1750	G
19	5	1754	U
19	5	1755	C
19	5	1756	U
19	5	1761	G
19	5	1764	G
19	5	1772	C
19	5	1773	U
19	5	1774	C
19	5	1776	A
19	5	1780	A
19	5	1781	U
19	5	1785	C
19	5	1787	A
19	5	1797	G
19	5	1800	U
19	5	1803	G
19	5	1804	A

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Mol	Chain	Res	Type
19	5	1805	A
19	5	1819	G
19	5	1821	G
19	5	1822	U
19	5	1828	C
19	5	1830	G
19	5	1834	U
19	5	1835	G
19	5	1836	G
19	5	1837	A
19	5	1842	G
19	5	1843	A
19	5	1850	A
19	5	1855	G
19	5	1863	U
19	5	1866	U
19	5	1869	G
19	5	1882	U
19	5	1886	G
19	5	1888	A
19	5	1892	A
19	5	1893	C
19	5	1897	A
19	5	1898	C
19	5	1910	G
19	5	1917	A
19	5	1918	U
19	5	1920	C
19	5	1921	C
19	5	1922	G
19	5	1925	G
19	5	1930	U
19	5	1931	C
19	5	1935	C
19	5	1945	G
19	5	1948	G
19	5	1951	G
19	5	1952	G
19	5	1957	U
19	5	1958	A
19	5	1959	U
19	5	1961	G

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Mol	Chain	Res	Type
19	5	1962	A
19	5	1964	A
19	5	1971	U
19	5	1976	G
19	5	1977	C
19	5	1978	C
19	5	1980	U
19	5	1983	A
19	5	1984	A
19	5	1985	G
19	5	1986	U
19	5	1987	C
19	5	1991	A
19	5	1993	C
19	5	1997	U
19	5	2001	G
19	5	2002	A
19	5	2003	G
19	5	2004	U
19	5	2011	C
19	5	2024	G
19	5	2025	A
19	5	2026	A
19	5	2034	G
19	5	2044	U
19	5	2046	G
19	5	2047	A
19	5	2048	U
19	5	2052	G
19	5	2055	G
19	5	2056	G
19	5	2062	C
19	5	2064	G
19	5	2069	A
19	5	2079	G
19	5	2084	U
19	5	2085	G
19	5	2089	G
19	5	2090	U
19	5	2092	G
19	5	2093	G
19	5	2094	C

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Mol	Chain	Res	Type
19	5	2095	A
19	5	2097	A
19	5	2098	G
19	5	2100	G
19	5	2101	A
19	5	2102	G
19	5	2104	A
19	5	2105	A
19	5	2106	G
19	5	2107	A
19	5	2108	G
19	5	2259	G
19	5	2260	C
19	5	2267	U
19	5	2268	A
19	5	2270	G
19	5	2273	G
19	5	2275	G
19	5	2289	C
19	5	2300	A
19	5	2301	G
19	5	2306	G
19	5	2313	A
19	5	2314	G
19	5	2325	C
19	5	2331	G
19	5	2332	A
19	5	2333	G
19	5	2345	G
19	5	2348	G
19	5	2351	C
19	5	2360	A
19	5	2364	G
19	5	2370	A
19	5	2377	C
19	5	2395	A
19	5	2399	G
19	5	2417	A
19	5	2422	C
19	5	2424	G
19	5	2425	U
19	5	2428	A

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Mol	Chain	Res	Type
19	5	2433	G
19	5	2436	U
19	5	2437	C
19	5	2440	U
19	5	2441	C
19	5	2447	U
19	5	2450	G
19	5	2453	A
19	5	2460	A
19	5	2469	C
19	5	2471	G
19	5	2474	G
19	5	2475	G
19	5	2485	U
19	5	2487	G
19	5	2488	C
19	5	2489	C
19	5	2490	U
19	5	2491	C
19	5	2503	G
19	5	2504	C
19	5	2505	C
19	5	2506	G
19	5	2513	A
19	5	2529	A
19	5	2530	U
19	5	2537	A
19	5	2546	G
19	5	2547	G
19	5	2549	G
19	5	2553	A
19	5	2566	G
19	5	2575	U
19	5	2583	C
19	5	2586	G
19	5	2587	A
19	5	2588	C
19	5	2591	A
19	5	2600	A
19	5	2601	A
19	5	2627	C
19	5	2631	U

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Mol	Chain	Res	Type
19	5	2638	G
19	5	2640	G
19	5	2653	C
19	5	2659	A
19	5	2661	U
19	5	2662	G
19	5	2669	C
19	5	2670	C
19	5	2673	G
19	5	2675	G
19	5	2686	G
19	5	2687	U
19	5	2689	C
19	5	2694	G
19	5	2695	A
19	5	2696	A
19	5	2707	U
19	5	2708	U
19	5	2709	C
19	5	2710	C
19	5	2711	G
19	5	2714	G
19	5	2715	G
19	5	2716	C
19	5	2725	A
19	5	2726	G
19	5	2735	G
19	5	2738	C
19	5	2740	U
19	5	2743	A
19	5	2744	A
19	5	2754	G
19	5	2759	G
19	5	2760	G
19	5	2763	U
19	5	2764	A
19	5	2769	U
19	5	2772	C
19	5	2787	A
19	5	2788	U
19	5	2790	U
19	5	2793	G

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Mol	Chain	Res	Type
19	5	2794	C
19	5	2795	A
19	5	2798	A
19	5	2801	U
19	5	2806	A
19	5	2807	A
19	5	2808	G
19	5	2814	C
19	5	2826	U
19	5	2827	G
19	5	2828	U
19	5	2838	G
19	5	2842	G
19	5	2845	A
19	5	2855	G
19	5	2897	G
19	5	2898	G
19	5	3601	C
19	5	3604	A
19	5	3605	C
19	5	3606	U
19	5	3616	U
19	5	3618	C
19	5	3619	G
19	5	3625	G
19	5	3626	G
19	5	3635	A
19	5	3636	C
19	5	3644	U
19	5	3646	A
19	5	3650	C
19	5	3662	A
19	5	3664	G
19	5	3670	C
19	5	3673	C
19	5	3674	G
19	5	3681	G
19	5	3691	G
19	5	3696	C
19	5	3711	A
19	5	3712	A
19	5	3729	U

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Mol	Chain	Res	Type
19	5	3737	A
19	5	3740	G
19	5	3747	A
19	5	3748	A
19	5	3753	G
19	5	3760	A
19	5	3763	A
19	5	3766	A
19	5	3767	C
19	5	3773	U
19	5	3774	A
19	5	3776	G
19	5	3777	G
19	5	3784	A
19	5	3786	U
19	5	3799	A
19	5	3810	C
19	5	3811	G
19	5	3812	C
19	5	3814	U
19	5	3817	A
19	5	3819	G
19	5	3822	U
19	5	3838	U
19	5	3839	G
19	5	3840	U
19	5	3843	C
19	5	3869	C
19	5	3877	A
19	5	3878	C
19	5	3879	G
19	5	3880	G
19	5	3889	G
19	5	3892	U
19	5	3897	G
19	5	3901	A
19	5	3902	A
19	5	3904	G
19	5	3905	A
19	5	3906	A
19	5	3907	G
19	5	3915	U

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Mol	Chain	Res	Type
19	5	3916	G
19	5	3918	G
19	5	3926	C
19	5	3927	U
19	5	3939	G
19	5	3943	A
19	5	4069	U
19	5	4070	U
19	5	4073	A
19	5	4076	G
19	5	4085	A
19	5	4086	G
19	5	4088	C
19	5	4092	G
19	5	4097	G
19	5	4116	C
19	5	4117	U
19	5	4118	U
19	5	4119	C
19	5	4120	U
19	5	4122	G
19	5	4127	A
19	5	4150	G
19	5	4158	C
19	5	4161	G
19	5	4163	U
19	5	4164	C
19	5	4171	C
19	5	4183	G
19	5	4184	G
19	5	4191	G
19	5	4201	G
19	5	4203	A
19	5	4212	A
19	5	4228	G
19	5	4229	U
19	5	4232	U
19	5	4233	A
19	5	4238	G
19	5	4249	G
19	5	4251	A
19	5	4254	G

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Mol	Chain	Res	Type
19	5	4255	A
19	5	4256	A
19	5	4257	A
19	5	4266	G
19	5	4267	G
19	5	4268	A
19	5	4271	A
19	5	4273	A
19	5	4278	C
19	5	4281	A
19	5	4282	A
19	5	4291	G
19	5	4296	U
19	5	4297	G
19	5	4304	A
19	5	4305	G
19	5	4306	U
19	5	4314	C
19	5	4317	A
19	5	4318	C
19	5	4323	A
19	5	4329	G
19	5	4330	G
19	5	4332	C
19	5	4338	G
19	5	4339	A
19	5	4349	C
19	5	4354	U
19	5	4355	G
19	5	4368	G
19	5	4373	G
19	5	4374	U
19	5	4376	A
19	5	4377	G
19	5	4378	A
19	5	4380	A
19	5	4382	G
19	5	4387	C
19	5	4393	G
19	5	4394	A
19	5	4395	U
19	5	4398	C

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Mol	Chain	Res	Type
19	5	4401	G
19	5	4411	G
19	5	4419	U
19	5	4420	U
19	5	4421	C
19	5	4422	A
19	5	4430	G
19	5	4436	U
19	5	4440	G
19	5	4444	C
19	5	4448	G
19	5	4449	A
19	5	4464	A
19	5	4471	U
19	5	4472	G
19	5	4475	G
19	5	4482	U
19	5	4488	A
19	5	4500	U
19	5	4510	A
19	5	4511	A
19	5	4512	U
19	5	4513	A
19	5	4515	G
19	5	4518	A
19	5	4519	C
19	5	4520	G
19	5	4523	A
19	5	4524	G
19	5	4531	U
19	5	4548	A
19	5	4549	G
19	5	4560	C
19	5	4567	G
19	5	4570	G
19	5	4573	G
19	5	4574	U
19	5	4575	G
19	5	4590	A
19	5	4599	A
19	5	4606	G
19	5	4608	G

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Mol	Chain	Res	Type
19	5	4626	A
19	5	4636	U
19	5	4637	G
19	5	4639	G
19	5	4656	A
19	5	4657	U
19	5	4661	G
19	5	4664	A
19	5	4670	C
19	5	4672	A
19	5	4677	U
19	5	4678	G
19	5	4687	A
19	5	4700	A
19	5	4709	U
19	5	4719	G
19	5	4720	C
19	5	4728	U
19	5	4736	C
19	5	4745	G
19	5	4747	C
19	5	4750	G
19	5	4751	G
19	5	4753	U
19	5	4754	G
19	5	4756	C
19	5	4757	C
19	5	4759	C
19	5	4761	G
19	5	4763	U
19	5	4764	A
19	5	4765	G
19	5	4771	C
19	5	4772	C
19	5	4776	G
19	5	4867	G
19	5	4870	G
19	5	4871	C
19	5	4872	G
19	5	4873	G
19	5	4874	A
19	5	4875	G

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Mol	Chain	Res	Type
19	5	4882	U
19	5	4883	C
19	5	4885	U
19	5	4891	G
19	5	4895	C
19	5	4904	G
19	5	4910	A
19	5	4911	A
19	5	4913	G
19	5	4914	G
19	5	4915	G
19	5	4918	C
19	5	4919	G
19	5	4920	C
19	5	4921	C
19	5	4922	C
19	5	4924	C
19	5	4925	U
19	5	4926	C
19	5	4928	C
19	5	4931	G
19	5	4934	A
19	5	4937	C
19	5	4938	A
19	5	4940	C
19	5	4943	A
19	5	4944	C
19	5	4948	C
19	5	4949	G
19	5	4950	U
19	5	4951	G
19	5	4956	A
19	5	4957	C
19	5	4958	C
19	5	4960	G
19	5	4963	G
19	5	4965	U
19	5	4966	A
19	5	4967	A
19	5	4976	U
19	5	4985	U
19	5	4988	U

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Mol	Chain	Res	Type
19	5	4989	U
19	5	4990	C
19	5	4991	U
19	5	4993	G
19	5	5014	A
19	5	5017	G
19	5	5041	G
19	5	5047	C
19	5	5050	C
19	5	5052	C
19	5	5053	U
19	5	5054	C
19	5	5056	A
19	5	5058	A
19	5	5061	A
19	5	5062	G
19	5	5067	U
21	7	7	G
21	7	25	G
21	7	42	A
21	7	53	U
21	7	54	A
21	7	64	G
21	7	74	A
21	7	76	U
21	7	97	G
21	7	100	A
21	7	109	U
21	7	110	G
21	7	111	C
21	7	120	U
22	8	2	G
22	8	34	U
22	8	35	C
22	8	38	U
22	8	59	A
22	8	62	A
22	8	63	U
22	8	75	G
22	8	79	G
22	8	86	U
22	8	87	G

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Mol	Chain	Res	Type
22	8	103	A
22	8	104	A
22	8	105	C
22	8	109	C
22	8	110	U
22	8	111	U
22	8	114	G
22	8	123	U
22	8	124	U
22	8	125	C
22	8	126	C
22	8	127	U
22	8	137	A
22	8	147	G
22	8	151	G
39	K	3	C
39	K	4	C
39	K	17	C
39	K	25	A
39	K	26	U
39	K	33	G
39	K	41	G
39	K	44	U
39	K	45	A
39	K	46	A
39	K	56	G
39	K	58	C
39	K	63	U
39	K	67	C
39	K	68	A
39	K	70	G
39	K	71	G
39	K	73	C
39	K	74	G
39	K	75	G
39	K	77	A
39	K	79	A
39	K	81	U
39	K	99	A
39	K	103	A
39	K	111	A
39	K	113	G

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Mol	Chain	Res	Type
39	K	115	U
39	K	124	U
39	K	126	G
39	K	127	C
39	K	129	C
39	K	130	G
39	K	141	A
39	K	142	C
39	K	143	U
39	K	146	G
39	K	147	A
39	K	154	U
39	K	155	G
39	K	158	A
39	K	162	C
39	K	163	U
39	K	167	G
39	K	168	C
39	K	178	C
39	K	180	G
39	K	182	C
39	K	183	G
39	K	184	G
39	K	187	G
39	K	188	C
39	K	190	G
39	K	191	A
39	K	192	C
39	K	202	G
39	K	213	G
39	K	215	G
39	K	289	G
39	K	290	U
39	K	292	A
39	K	294	U
39	K	304	C
39	K	305	U
39	K	307	G
39	K	308	G
39	K	309	G
39	K	312	G
39	K	314	U

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Mol	Chain	Res	Type
39	K	318	A
39	K	319	C
39	K	323	C
39	K	332	G
39	K	339	A
39	K	347	G
39	K	350	C
39	K	351	G
39	K	360	A
39	K	362	C
39	K	364	A
39	K	368	U
39	K	369	C
39	K	370	G
39	K	372	U
39	K	381	C
39	K	382	C
39	K	385	G
39	K	386	C
39	K	398	A
39	K	400	C
39	K	408	A
39	K	409	C
39	K	417	C
39	K	418	A
39	K	428	U
39	K	435	A
39	K	438	G
39	K	441	C
39	K	448	A
39	K	449	A
39	K	450	C
39	K	464	A
39	K	465	A
39	K	466	G
39	K	471	G
39	K	472	C
39	K	473	A
39	K	474	G
39	K	482	G
39	K	487	U
39	K	492	C

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Mol	Chain	Res	Type
39	K	496	C
39	K	525	A
39	K	530	U
39	K	531	A
39	K	532	C
39	K	533	A
39	K	544	G
39	K	548	C
39	K	549	C
39	K	550	C
39	K	551	U
39	K	554	A
39	K	555	A
39	K	556	U
39	K	559	G
39	K	560	A
39	K	563	G
39	K	564	A
39	K	568	C
39	K	570	C
39	K	573	U
39	K	576	A
39	K	583	A
39	K	587	A
39	K	588	G
39	K	589	G
39	K	590	A
39	K	591	U
39	K	600	G
39	K	603	C
39	K	604	A
39	K	605	A
39	K	606	G
39	K	608	C
39	K	614	C
39	K	617	G
39	K	627	U
39	K	628	A
39	K	629	A
39	K	631	U
39	K	632	C
39	K	643	A

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Mol	Chain	Res	Type
39	K	644	G
39	K	655	A
39	K	659	G
39	K	660	C
39	K	662	G
39	K	668	A
39	K	669	A
39	K	670	A
39	K	671	A
39	K	672	A
39	K	684	G
39	K	687	C
39	K	688	U
39	K	689	U
39	K	690	G
39	K	752	G
39	K	753	C
39	K	754	G
39	K	798	G
39	K	799	U
39	K	810	A
39	K	811	A
39	K	812	A
39	K	818	A
39	K	821	G
39	K	822	U
39	K	830	A
39	K	834	C
39	K	847	A
39	K	867	G
39	K	868	G
39	K	869	A
39	K	870	A
39	K	871	U
39	K	872	A
39	K	873	G
39	K	874	G
39	K	875	A
39	K	878	G
39	K	887	U
39	K	888	U
39	K	890	U

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Mol	Chain	Res	Type
39	K	892	U
39	K	903	A
39	K	906	U
39	K	907	G
39	K	913	A
39	K	914	U
39	K	918	U
39	K	920	A
39	K	930	C
39	K	933	G
39	K	934	G
39	K	943	U
39	K	958	G
39	K	971	G
39	K	989	C
39	K	990	A
39	K	992	A
39	K	999	G
39	K	1002	U
39	K	1009	A
39	K	1017	U
39	K	1023	A
39	K	1041	G
39	K	1050	A
39	K	1058	A
39	K	1060	A
39	K	1062	A
39	K	1067	C
39	K	1083	A
39	K	1085	C
39	K	1089	G
39	K	1100	A
39	K	1109	C
39	K	1113	A
39	K	1114	U
39	K	1115	U
39	K	1116	C
39	K	1117	C
39	K	1118	C
39	K	1123	C
39	K	1131	G
39	K	1133	A

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Mol	Chain	Res	Type
39	K	1138	C
39	K	1139	C
39	K	1148	A
39	K	1153	C
39	K	1154	U
39	K	1155	U
39	K	1170	A
39	K	1195	A
39	K	1207	G
39	K	1208	A
39	K	1215	C
39	K	1220	A
39	K	1224	G
39	K	1240	A
39	K	1242	U
39	K	1245	G
39	K	1251	A
39	K	1253	A
39	K	1256	G
39	K	1257	G
39	K	1259	A
39	K	1265	A
39	K	1271	C
39	K	1274	G
39	K	1275	G
39	K	1280	G
39	K	1281	G
39	K	1282	A
39	K	1284	A
39	K	1285	G
39	K	1286	G
39	K	1291	A
39	K	1293	A
39	K	1295	A
39	K	1299	A
39	K	1301	A
39	K	1302	G
39	K	1303	C
39	K	1307	U
39	K	1308	U
39	K	1310	U
39	K	1313	A

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Mol	Chain	Res	Type
39	K	1314	U
39	K	1315	U
39	K	1316	C
39	K	1322	G
39	K	1341	C
39	K	1342	U
39	K	1348	G
39	K	1371	U
39	K	1372	U
39	K	1376	A
39	K	1378	A
39	K	1382	A
39	K	1384	C
39	K	1386	A
39	K	1395	C
39	K	1396	A
39	K	1397	U
39	K	1401	A
39	K	1402	A
39	K	1404	U
39	K	1410	C
39	K	1411	G
39	K	1428	G
39	K	1429	G
39	K	1439	A
39	K	1454	A
39	K	1459	G
39	K	1462	U
39	K	1463	U
39	K	1466	G
39	K	1473	G
39	K	1476	A
39	K	1477	U
39	K	1478	U
39	K	1480	A
39	K	1487	A
39	K	1488	C
39	K	1489	A
39	K	1490	G
39	K	1497	G
39	K	1498	A
39	K	1507	G

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Mol	Chain	Res	Type
39	K	1509	U
39	K	1510	G
39	K	1521	C
39	K	1522	A
39	K	1523	C
39	K	1531	A
39	K	1533	A
39	K	1544	C
39	K	1548	G
39	K	1552	G
39	K	1553	C
39	K	1554	C
39	K	1555	U
39	K	1556	A
39	K	1557	C
39	K	1560	U
39	K	1570	G
39	K	1575	G
39	K	1580	A
39	K	1581	C
39	K	1585	U
39	K	1586	U
39	K	1587	G
39	K	1588	A
39	K	1598	G
39	K	1601	A
39	K	1604	G
39	K	1621	U
39	K	1623	A
39	K	1625	U
39	K	1637	A
39	K	1638	G
39	K	1648	G
39	K	1654	G
39	K	1664	A
39	K	1665	G
39	K	1671	G
39	K	1680	G
39	K	1683	C
39	K	1695	A
39	K	1698	C
39	K	1699	A

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Mol	Chain	Res	Type
39	K	1701	C
39	K	1715	A
39	K	1721	U
39	K	1722	G
39	K	1726	G
39	K	1744	G
39	K	1746	U
39	K	1748	G
39	K	1753	C
39	K	1757	G
39	K	1758	G
39	K	1783	C
39	K	1785	C
39	K	1800	A
39	K	1823	A
39	K	1825	A
39	K	1826	G
39	K	1829	G
39	K	1831	A
39	K	1836	G
39	K	1837	G
39	K	1838	U
39	K	1845	A
39	K	1849	G
39	K	1851	A
39	K	1852	C
39	K	1859	A
39	K	1861	G
39	K	1862	G
39	K	1863	A
39	K	1865	C
39	K	1866	A
39	K	1867	U
39	K	1869	A

All (101) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
16	2	20	C
16	2	60	A
19	5	48	G
19	5	125	C

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Mol	Chain	Res	Type
19	5	134	G
19	5	217	C
19	5	224	U
19	5	245	C
19	5	265	C
19	5	275	C
19	5	406	C
19	5	408	A
19	5	449	C
19	5	480	C
19	5	485	C
19	5	492	U
19	5	504	G
19	5	685	C
19	5	696	C
19	5	922(B)	C
19	5	930	G
19	5	959	G
19	5	966	A
19	5	971(A)	G
19	5	1072	C
19	5	1174	G
19	5	1211	G
19	5	1236	C
19	5	1238	A
19	5	1291	G
19	5	1329	G
19	5	1370	G
19	5	1440	U
19	5	1445	U
19	5	1455	G
19	5	1563	A
19	5	1633	G
19	5	1804	A
19	5	1818	G
19	5	1834	U
19	5	1921	C
19	5	1979	A
19	5	1983	A
19	5	2046	G
19	5	2068	C
19	5	2089	G

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Mol	Chain	Res	Type
19	5	2266	C
19	5	2468	U
19	5	2474	G
19	5	2502	A
19	5	2513	A
19	5	2529	A
19	5	2546	G
19	5	2587	A
19	5	2661	U
19	5	2695	A
19	5	3625	G
19	5	3765	G
19	5	3876	A
19	5	3888	G
19	5	3904	G
19	5	4119	C
19	5	4170	A
19	5	4232	U
19	5	4254	G
19	5	4354	U
19	5	4448	G
19	5	4464	A
19	5	4510	A
19	5	4699	U
19	5	4719	G
19	5	4884	G
19	5	4925	U
19	5	4936	G
19	5	4947	U
22	8	124	U
39	K	110	U
39	K	182	C
39	K	369	C
39	K	434	G
39	K	465	A
39	K	532	C
39	K	553	U
39	K	642	U
39	K	688	U
39	K	752	G
39	K	870	A
39	K	872	A

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Mol	Chain	Res	Type
39	K	874	G
39	K	912	C
39	K	1061	U
39	K	1114	U
39	K	1137	U
39	K	1394	G
39	K	1395	C
39	K	1396	A
39	K	1489	A
39	K	1520	G
39	K	1637	A
39	K	1664	A
39	K	1824	A

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 305 ligands modelled in this entry, 305 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
19	5	24
39	K	11
86	XX	6
17	3	2
22	8	1
16	2	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	5	2113:G	O3'	2258:C	P	41.14
1	5	1252:C	O3'	1271:G	P	36.47
1	5	1219:G	O3'	1233:G	P	20.39
1	K	697:G	O3'	729:C	P	18.51
1	5	3948:C	O3'	4065:G	P	18.39
1	K	834:C	O3'	841:G	P	18.02
1	K	756:C	O3'	788:G	P	17.51
1	5	523:C	O3'	638:G	P	17.16
1	5	990:C	O3'	1064:G	P	17.06
1	K	1761:U	O3'	1771:G	P	17.03
1	5	4101:C	O3'	4107:G	P	16.93
1	K	323:C	O3'	329:G	P	16.68
1	5	4777:C	O3'	4859:C	P	16.43
1	5	4138:C	O3'	4146:G	P	16.19
1	K	1417:C	O3'	1423:C	P	15.71
1	K	130:G	O3'	140:U	P	15.19
1	5	5022:U	O3'	5028:G	P	14.70
1	5	1696:C	O3'	1720:C	P	14.56
1	5	2901:G	O3'	3597:G	P	13.53
1	5	760:G	O3'	904:C	P	13.50
1	5	1364:U	O3'	1368:A	P	13.46
1	5	182:G	O3'	189:G	P	13.44
1	8	79:G	O3'	85:U	P	12.67
1	5	512:U	O3'	515:C	P	10.15
1	5	1180:C	O3'	1183:C	P	9.83
1	5	4729:A	O3'	4735:G	P	9.21
1	K	225:G	O3'	287:U	P	8.51
1	K	745:C	O3'	749:U	P	8.30
1	XX	133:MET	C	145:SER	N	7.02
1	K	736:C	O3'	743:U	P	6.46

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	5	500:G	O3'	504:G	P	5.93
1	2	16:C	O3'	18:G	P	5.89
1	3	19:G	O3'	20:U	P	5.81
1	5	1100:U	O3'	1168:G	P	5.29
1	5	4740:G	O3'	4743:G	P	5.03
1	5	1239:C	O3'	1244:G	P	5.01
1	K	1432:U	O3'	1438:A	P	4.66
1	5	1438:U	O3'	1440:U	P	4.07
1	3	16:C	O3'	18:U	P	3.95
1	XX	101:GLU	C	102:VAL	N	3.60
1	5	4899:G	O3'	4902:C	P	3.56
1	XX	77:MET	C	78:GLU	N	2.76
1	XX	442:GLY	C	443:SER	N	2.47
1	XX	439:GLY	C	440:ALA	N	2.23
1	XX	107:LYS	C	108:ASP	N	1.94

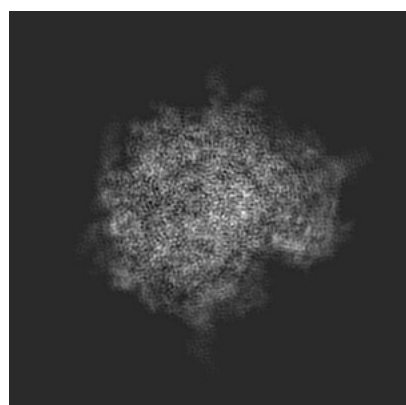
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4745. These allow visual inspection of the internal detail of the map and identification of artifacts.

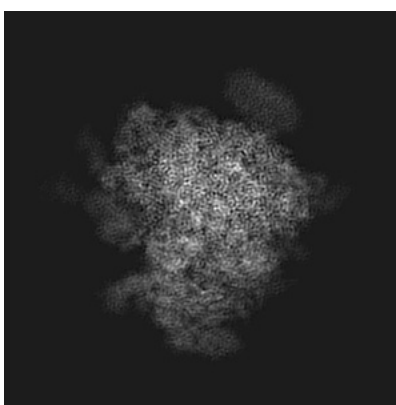
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

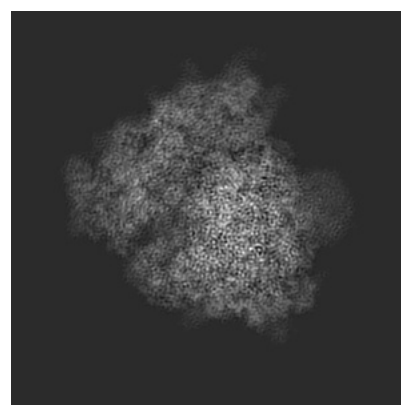
6.1.1 Primary map



X



Y

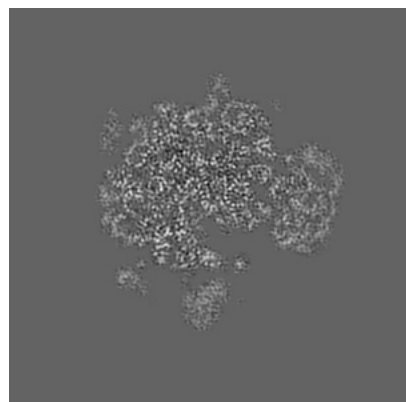


Z

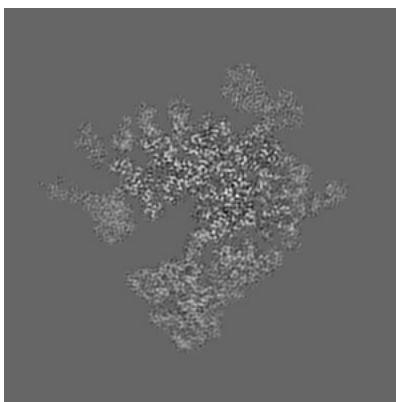
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

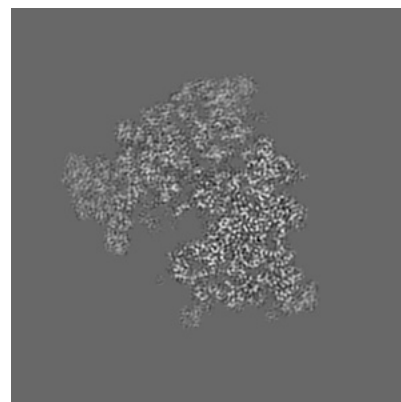
6.2.1 Primary map



X Index: 198



Y Index: 198

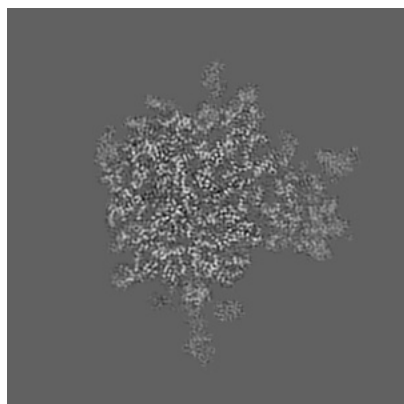


Z Index: 198

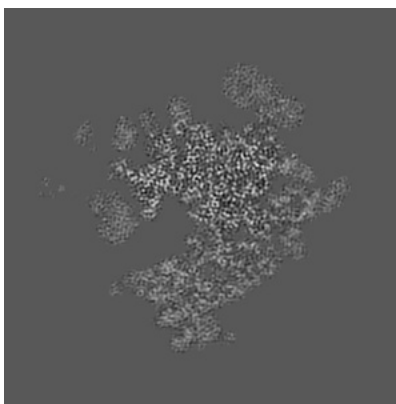
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

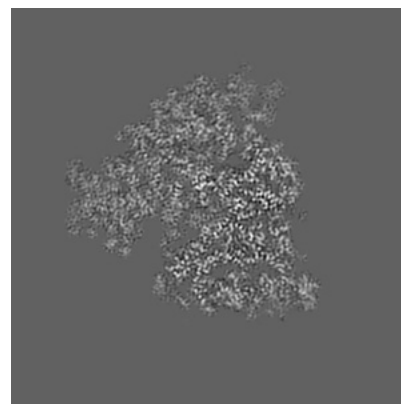
6.3.1 Primary map



X Index: 215



Y Index: 204

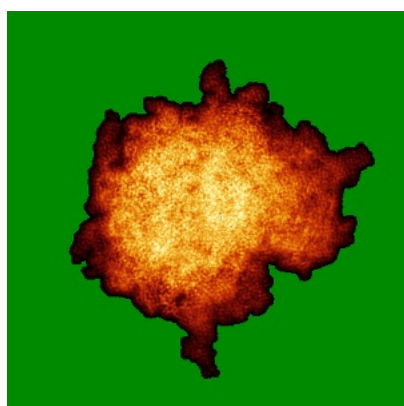


Z Index: 191

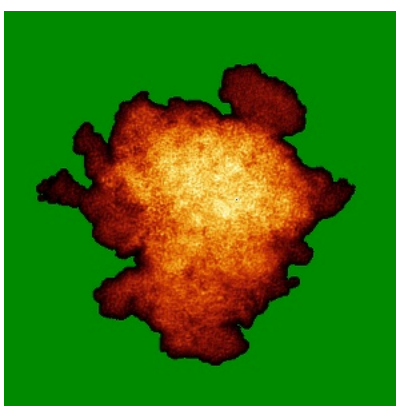
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

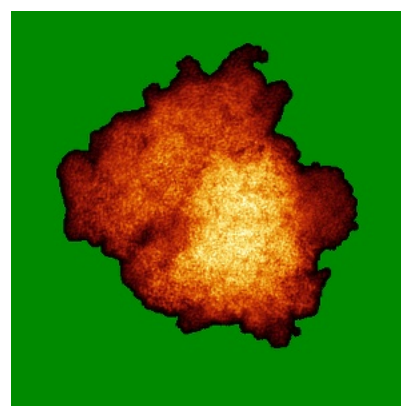
6.4.1 Primary map



X



Y

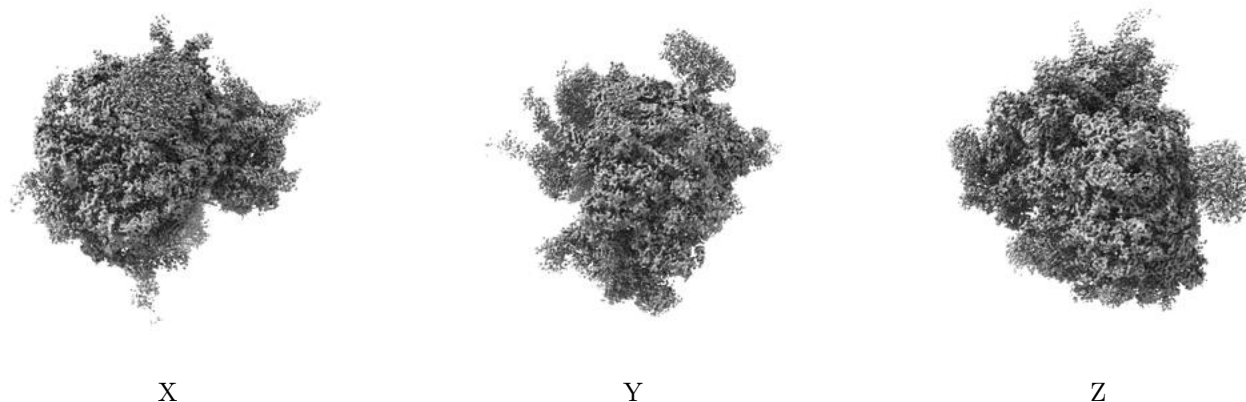


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.08. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

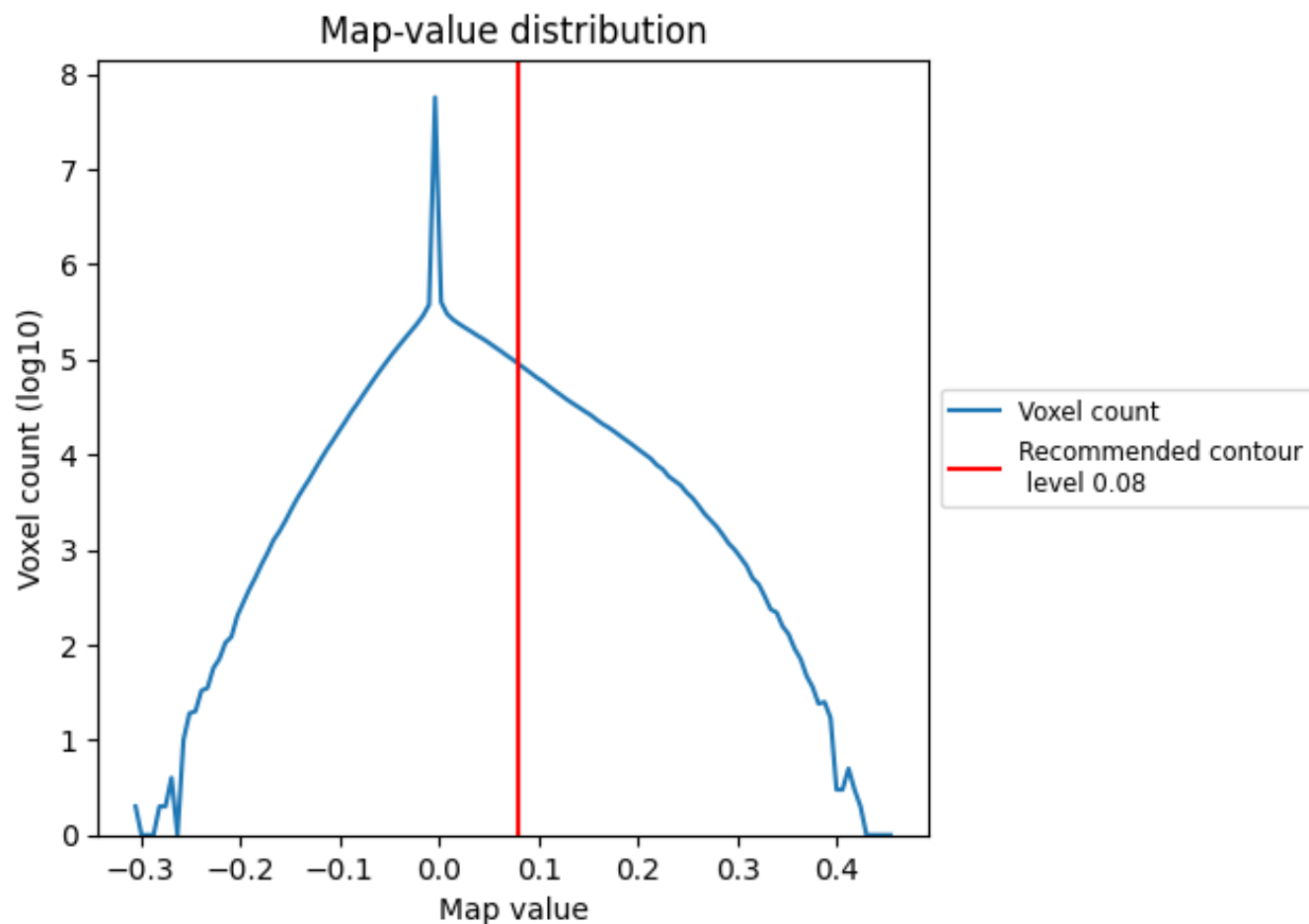
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

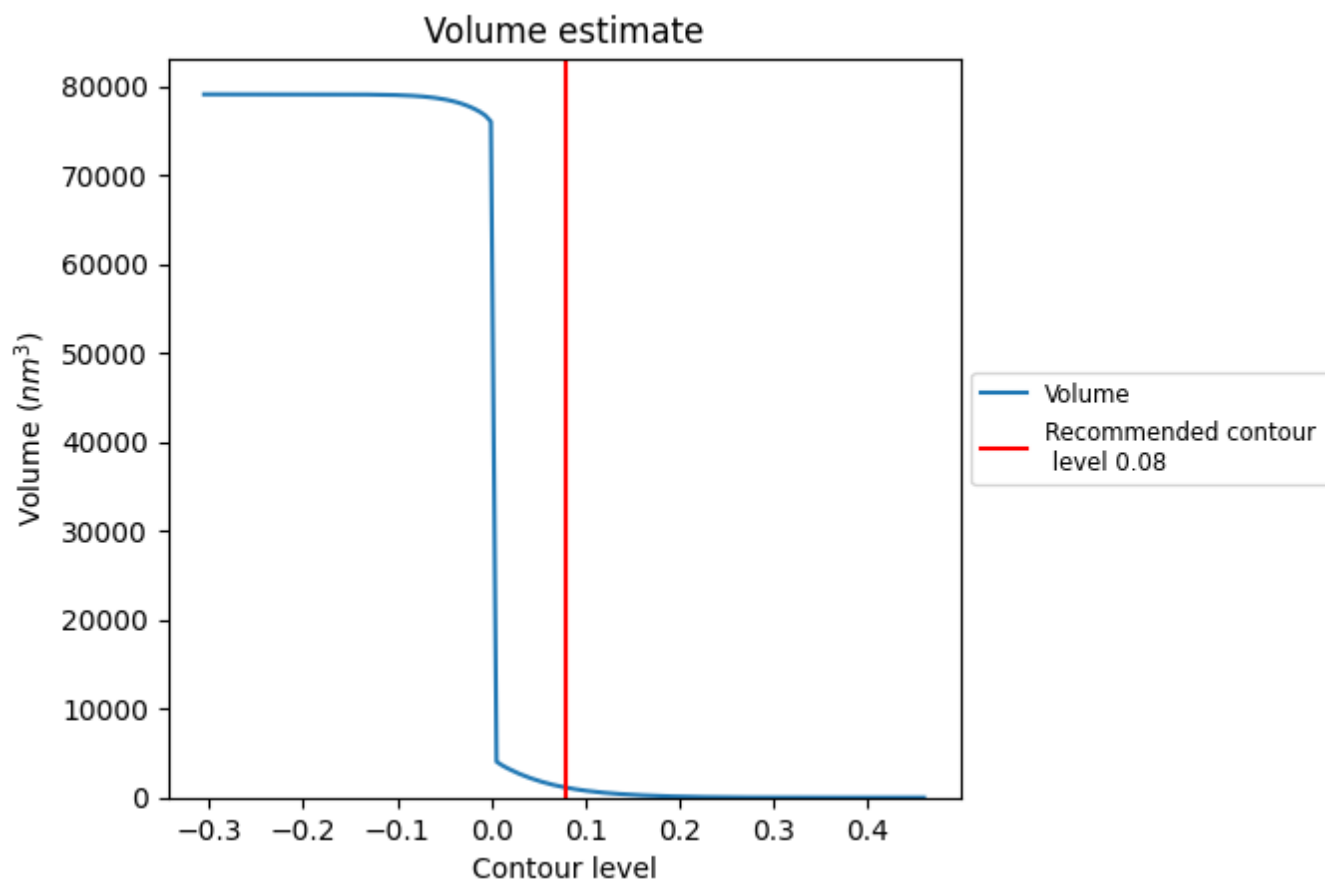
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

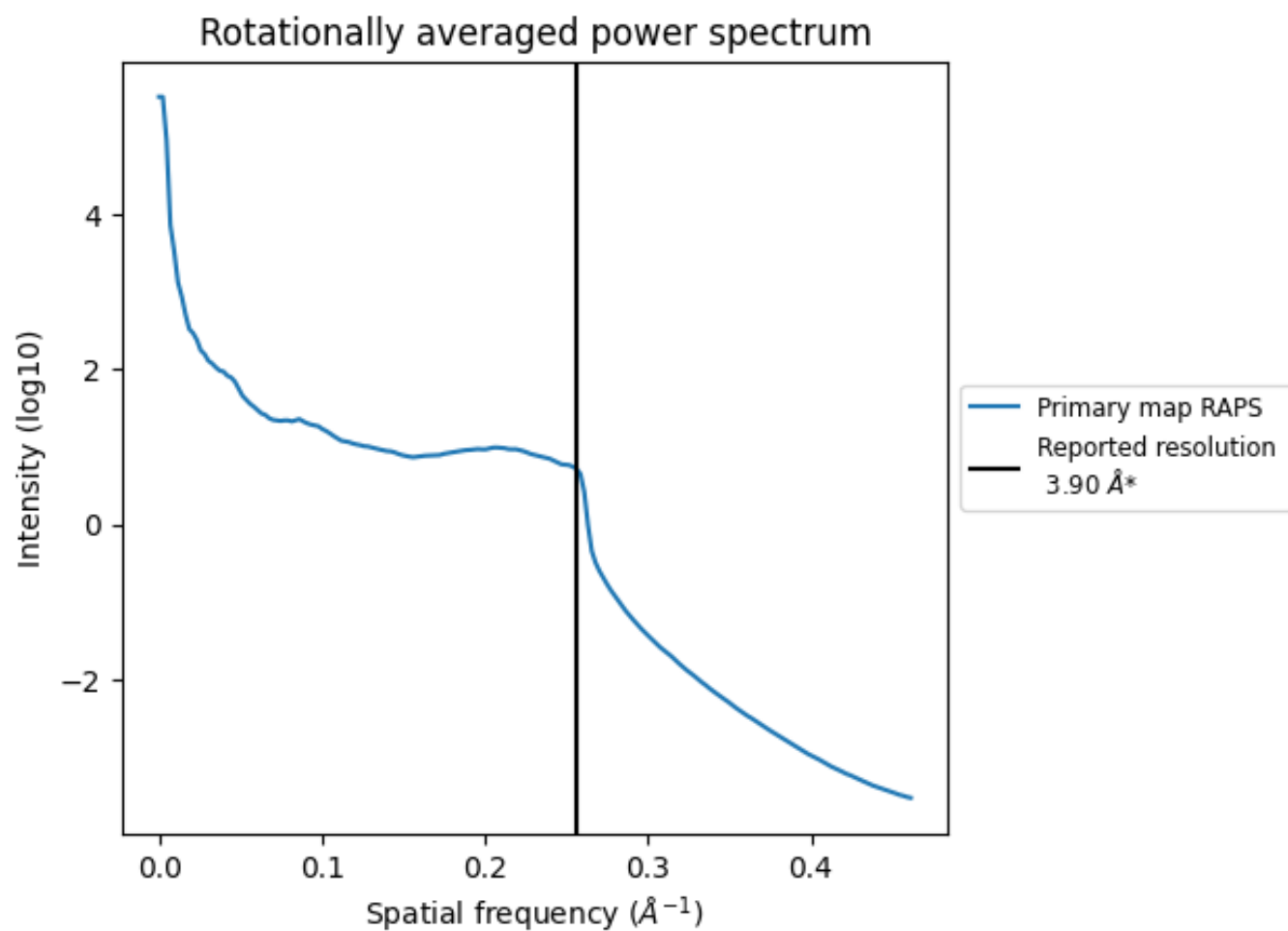
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 11111 nm³; this corresponds to an approximate mass of 1003 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

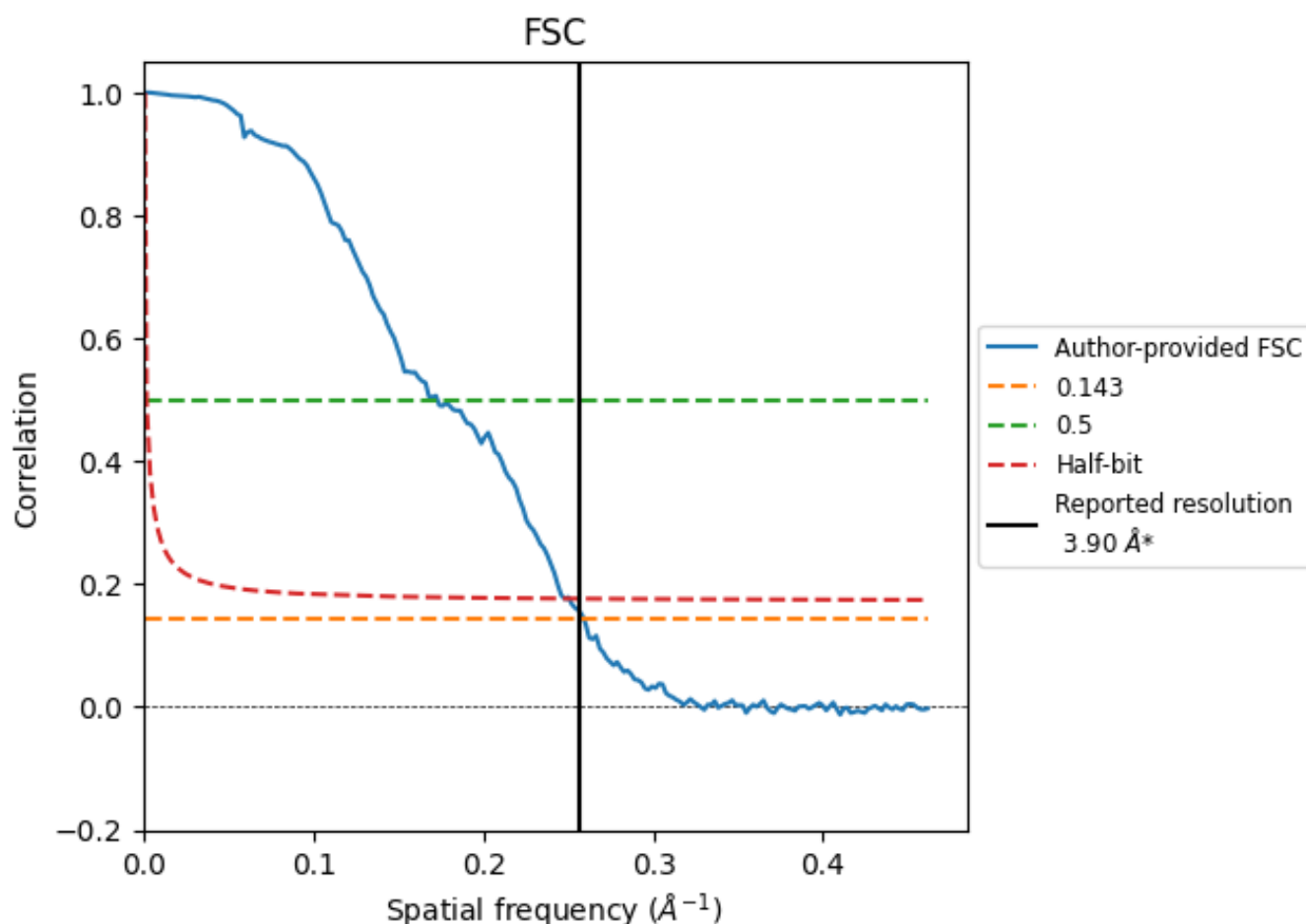


*Reported resolution corresponds to spatial frequency of 0.256 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.256 Å⁻¹

8.2 Resolution estimates [i](#)

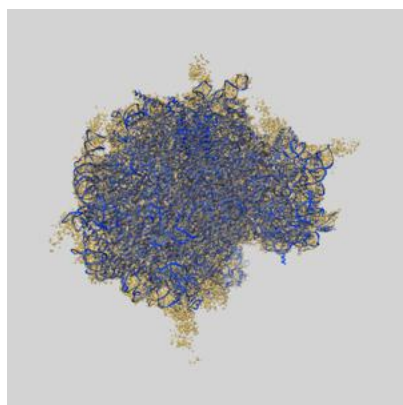
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	3.86	5.78	4.03
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

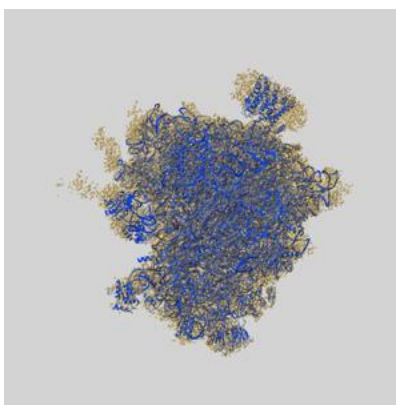
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-4745 and PDB model 6R7Q. Per-residue inclusion information can be found in [section 3](#) on [page 23](#).

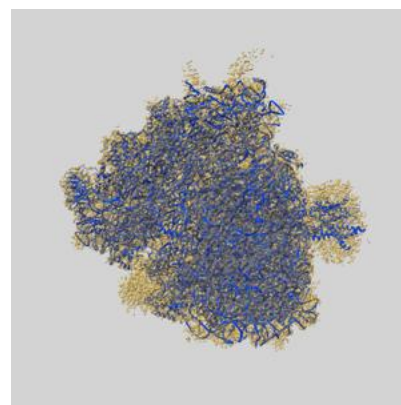
9.1 Map-model overlay [i](#)



X



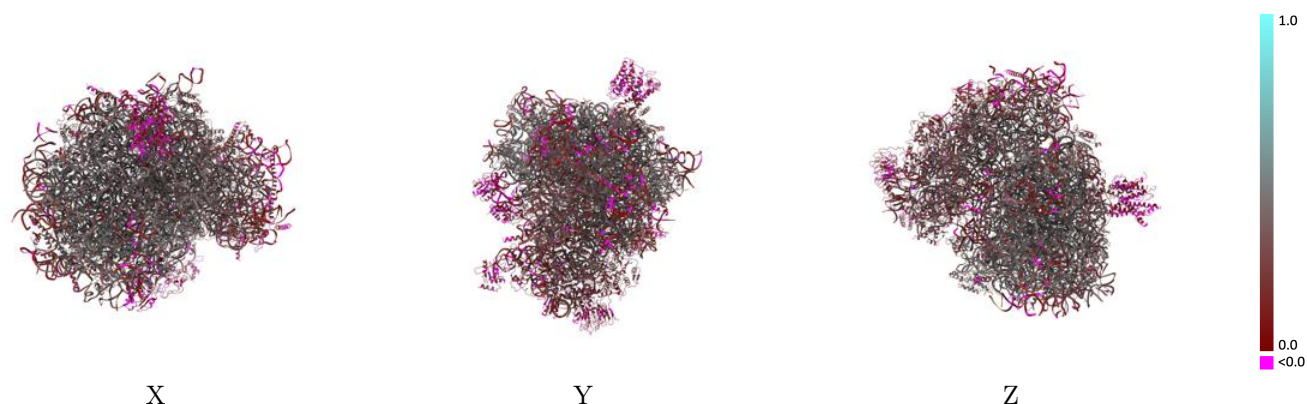
Y



Z

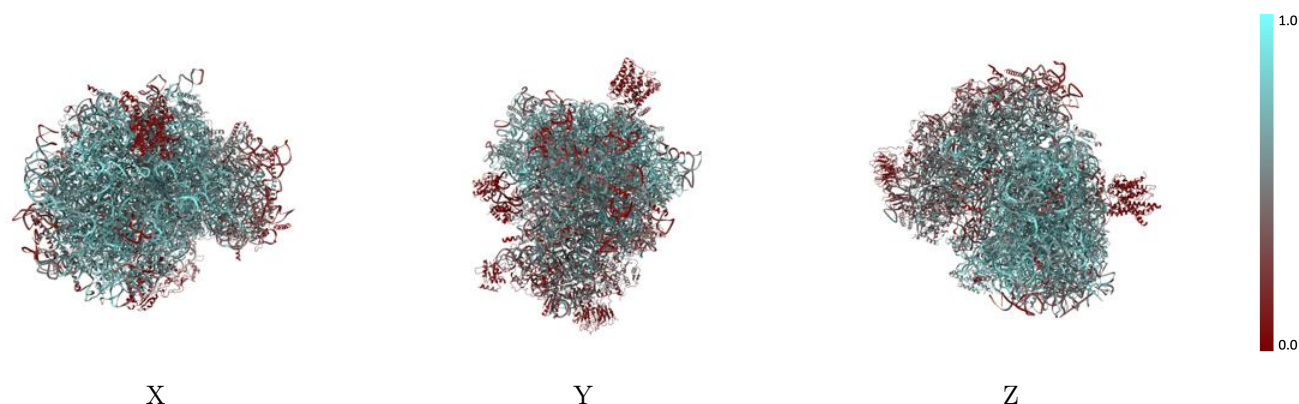
The images above show the 3D surface view of the map at the recommended contour level 0.08 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



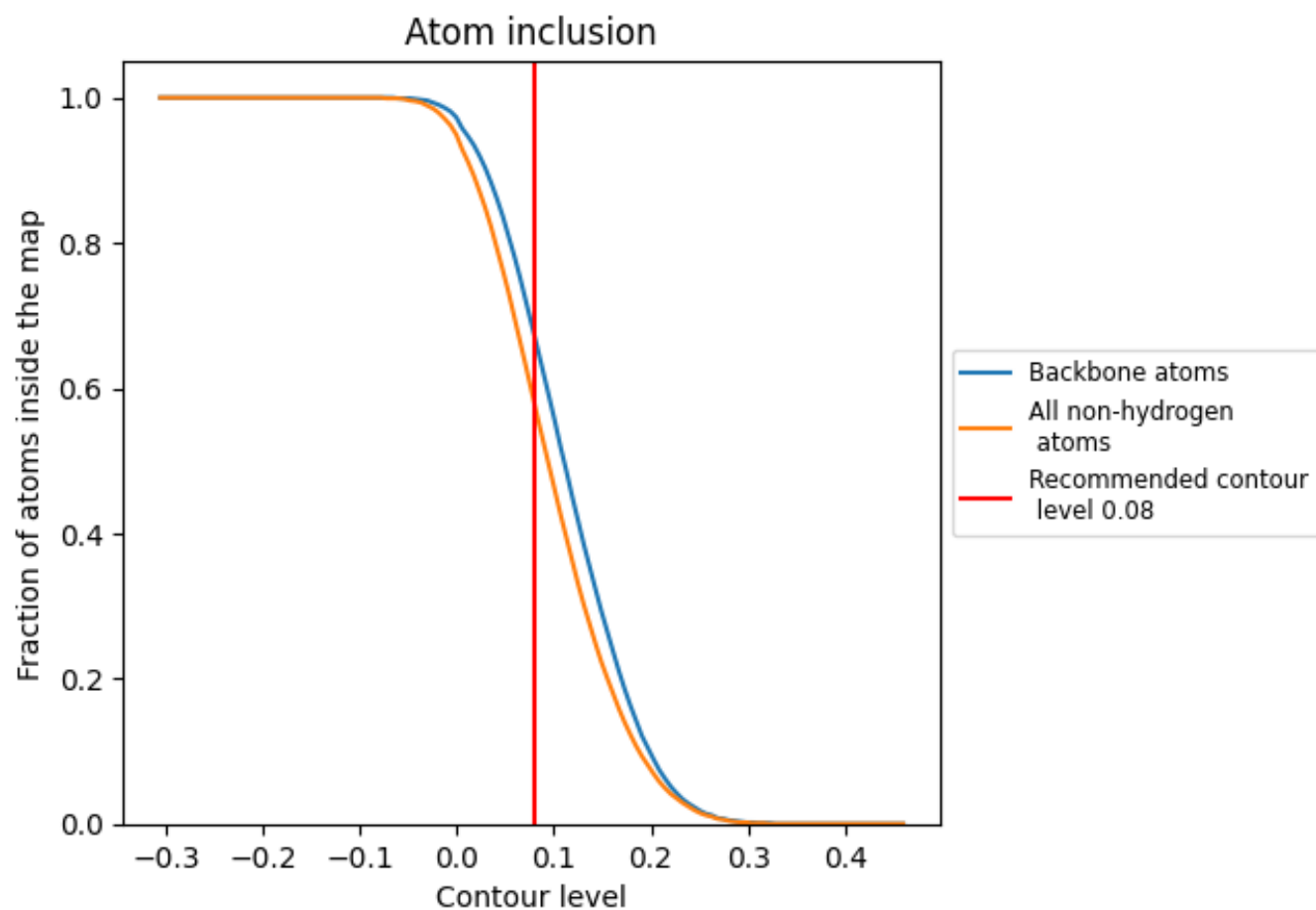
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.08).

9.4 Atom inclusion [i](#)



At the recommended contour level, 67% of all backbone atoms, 58% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5780	 0.3400
0	 0.1760	 0.1040
1	 0.3220	 0.4330
2	 0.3340	 0.2960
3	 0.2930	 0.1640
4	 0.3390	 0.2880
5	 0.7010	 0.3720
6	 0.1490	 0.1330
7	 0.7970	 0.4190
8	 0.7300	 0.3840
9	 0.4150	 0.3180
A	 0.6390	 0.4340
AA	 0.3070	 0.2330
B	 0.6480	 0.4220
BB	 0.3580	 0.2450
C	 0.6450	 0.4320
CC	 0.4470	 0.3300
D	 0.6060	 0.3800
DD	 0.3710	 0.2580
E	 0.5530	 0.3860
EE	 0.4820	 0.3610
F	 0.6040	 0.4130
FF	 0.3190	 0.2800
G	 0.5440	 0.3470
GG	 0.2530	 0.1790
H	 0.6130	 0.3950
HH	 0.3600	 0.2930
I	 0.6100	 0.4150
II	 0.3970	 0.2740
J	 0.5930	 0.3740
JJ	 0.4290	 0.2860
K	 0.5880	 0.3130
KK	 0.3390	 0.2560
L	 0.6090	 0.3820
LL	 0.4810	 0.3380



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Chain	Atom inclusion	Q-score
M	 0.6370	 0.4130
MM	 0.4770	 0.3470
N	 0.6800	 0.4340
NN	 0.3210	 0.2400
O	 0.6620	 0.4220
OO	 0.3960	 0.2500
P	 0.6480	 0.4360
PP	 0.3480	 0.2300
Q	 0.6360	 0.4320
QQ	 0.5050	 0.3570
R	 0.5840	 0.3650
RR	 0.1330	 0.0970
S	 0.6580	 0.4410
SS	 0.2850	 0.2010
T	 0.5990	 0.4100
TT	 0.4430	 0.3440
U	 0.5250	 0.3240
UU	 0.3310	 0.2460
V	 0.6280	 0.4260
VV	 0.4710	 0.3640
W	 0.4080	 0.2810
WW	 0.3440	 0.2270
X	 0.6120	 0.3900
XX	 0.1230	 0.0920
Y	 0.6210	 0.3910
YY	 0.1230	 0.1000
Z	 0.6040	 0.3780
ZZ	 0.0490	 0.0370
a	 0.6620	 0.4470
b	 0.4240	 0.3220
c	 0.5600	 0.3640
d	 0.5950	 0.3920
e	 0.6320	 0.4420
f	 0.6640	 0.4550
g	 0.6020	 0.4040
h	 0.6090	 0.3760
i	 0.5970	 0.3500
j	 0.6650	 0.4390
k	 0.5280	 0.3480
l	 0.5860	 0.4060
m	 0.6370	 0.4030
n	 0.5960	 0.3640

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Chain	Atom inclusion	Q-score
o	 0.5990	 0.4160
p	 0.6010	 0.4010
q	 0.4050	 0.2870
r	 0.6250	 0.4290
s	 0.0600	 0.0260
t	 0.0160	 0.0130
u	 0.4530	 0.3290
v	 0.4510	 0.3160
w	 0.2850	 0.2200
x	 0.3640	 0.2840
y	 0.3610	 0.2740
z	 0.3060	 0.2220